* * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 15:37:17 ON 08 SEP 2005

=> file reg

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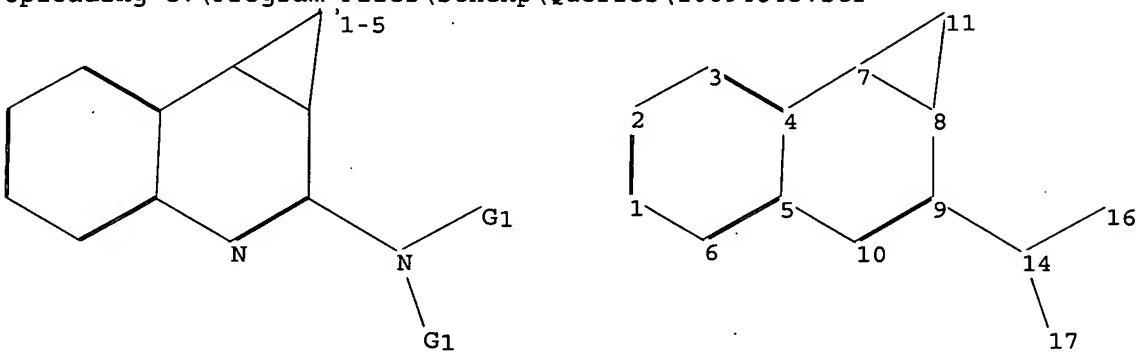

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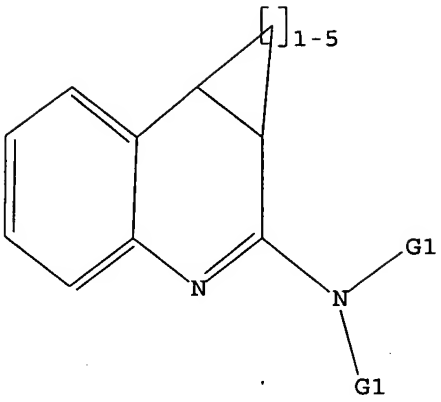
14 16 17
ring nodes :
1 2 3 4 5 6 7 8 9 10 11
chain bonds :
9-14 14-16 14-17
ring bonds :
1-2 1-6 2-3 3-4 4-5 4-7 5-6 5-10 7-8 7-11 8-9 8-11 9-10
exact/norm bonds :
4-7 5-10 7-8 7-11 8-9 8-11 9-10 9-14 14-16 14-17
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6

G1:C,H,O,N

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 14:CLASS 16:CLASS 17:CLASS

L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR



G1 C,H,O,N

Structure attributes must be viewed using STN Express query preparation.

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L3          666 SEA SSS FUL L1

=> file ca


=> s l3
L4          151 L3

=> s l4 an py<1999
MISSING OPERATOR L4 AN
The search profile that was entered contains terms or
nested terms that are not separated by a logical operator.

=> s l4 and py<1999
      18655783 PY<1999
L5           90 L4 AND PY<1999

=> s l5 and (pharm? or drug?)
         522458 PHARM?
         730437 DRUG?
L6           12 L5 AND (PHARM? OR DRUG?)

=> d ibib abs fhitstr 1-12
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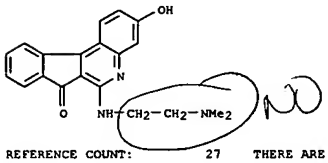
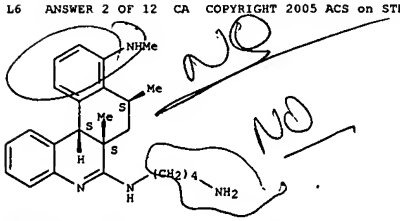
L6 ANSWER 1 OF 12 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 129:183768 CA
TITLE: TAS-103: antineoplastic topoisomerase I and II inhibitor
AUTHOR(S): Hoshi, A.; Castaner, J.
CORPORATE SOURCE: Tokyo, 125, Japan
SOURCE: Drugs of the Future (1998), 23(5), 513-515
CODEN: DRFUD4; ISSN: 0377-8282
PUBLISHER: Prous Science
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English
AB A brief review with 24 refs., describing synthesis, pharmacol. actions, mechanism of action, toxicity, and clin. studies of the indeno[2,1-c]-quinolin-7-one derivative TAS-103, an antineoplastic topoisomerase I and II inhibitor.
IT **174634-08-3P**, 7H-Indeno[2,1-c]quinolin-7-one, 6-[[2-(dimethylamino)ethyl]amino]-3-hydroxy-
RL: BAC (Biological activity or effector, except adverse); BPN (Biosynthetic preparation); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(TAS-103, antineoplastic topoisomerase I and II inhibitor)
RN 174634-08-3 CA
CN 7H-Indeno[2,1-c]quinolin-7-one, 6-[[2-(dimethylamino)ethyl]amino]-3-hydroxy- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 2 OF 12 CA COPYRIGHT 2005 ACS on STN (Continued)



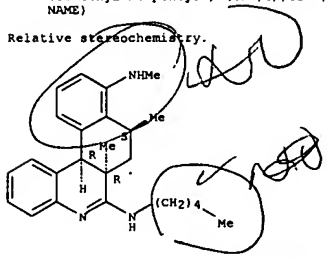
REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 2 OF 12 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 128:265841 CA
TITLE: Inhibition of tumor growth and polyamine uptake by tetracyclic amidines bearing a putrescine moiety
AUTHOR(S): Mens, T.; Tomasi, S.; Eifler-Lima, V. L.; Uriac, P.; Huet, J.; Catros-Quemener, V.
CORPORATE SOURCE: Groupe de Recherche en Therapeutique Anticancereuse, UPRES-A CNRS 6027, Faculte de Medecine de Rennes, Rennes, 35043, Fr.
SOURCE: Anticancer Research (1997), 17(6D), 4327-4332
CODEN: ANTRD4; ISSN: 0250-7005
PUBLISHER: Anticancer Research
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Tetracyclic amidines (tetrahydroquino[4.3-b][1]benzazepine (I) and tetrahydrobenzo[k]naphthyridine (II)) bearing a putrescine moiety possess significant DNA-binding affinity. The authors report here that these compds. and their a and b isomers inhibit tumor cell growth and putrescine uptake in 3LL carcinoma cells in vitro. Moreover, I reduced by 50% the accumulation of putrescine in intestinal brush border membrane vesicles. In CHO-MG, a cell line deficient for the specific polyamine uptake system, the cytotoxicity of these compds. was significantly reduced compared to the CHO wild cell line. The IC50 for CHO-MG was significantly higher than for CHO, demonstrating that the polyamine transport system increased the efficacy of these compds. The efficacy of I and II might therefore be related to their ability to interact with DNA as well as their structural analogy with polyamines. Moreover, the authors clearly show that DFMO enhances the efficacy of these tetracyclic amidines in vivo. Potential mechanisms include: (a) lower intracellular polyamine levels reduces polyamine DNA-stabilizing functions, increasing accessibility for DNA-binding drugs; (b) DFMO enhances the polyamine uptake system in tumor cells, increasing the entry of tetracyclic amidines bearing a putrescine moiety as well as their accessibility to final DNA-binding sites. The fact that natural polyamine uptake is reduced by the same compds. constitutes an additive mechanism for antitumoral efficiency.
IT **205697-81-0**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(inhibition of tumor growth and polyamine uptake by tetracyclic amidines bearing a putrescine moiety)
RN 205697-81-0 CA
CN Benzo[k]phenanthridine-6,9-diamine, N6-(4-aminobutyl)-6a,7,8,12b-tetrahydro-N9,6a,8-trimethyl-, (6aα,8α,12bα)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L6 ANSWER 3 OF 12 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 127:257203 CA
TITLE: Depletion of polyamines potentiates the antitumor effect of tetracyclic amidines bearing a putrescine moiety
AUTHOR(S): Tomasi, S.; Eifler-Lima, V. L.; Le Roch, M.; Corbel, J. C.; Renault, J.; Uriac, P.; Mens, T.; Catros-Quemener, V.; Moulinoux, J. P.
CORPORATE SOURCE: UPRES de Pharmacochimie de Molecules de Synthese et de Substances Naturelles, Faculte de Pharmacie, Rennes, 35043, Fr.
SOURCE: Pharmaceutical Sciences (1997), 3(5/6), 241-247
CODEN: PHSCFB; ISSN: 1356-6881
PUBLISHER: Royal Pharmaceutical Society of Great Britain
DOCUMENT TYPE: Journal
LANGUAGE: English
AB D,L-2-(difluoromethyl)ornithine (DFMO), a potent inactivator of putrescine biosynthesis that depletes spermidine levels in cells, is known to enhance cytotoxicity of DNA-binding drugs. A significant in-vitro cytotoxicity and DNA-binding affinity found for amidines containing both heterocyclic and polyamine moieties prompted the authors to evaluate their in-vivo activity on Lewis lung carcinoma (3LL). When administered alone to tumor bearing mice, neither DFMO nor the tetracyclic amidines were effective. However, their combined administration with DFMO inhibited tumor growth significantly.
IT **196296-15-8P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(depletion of polyamines with DFMO potentiates antitumor effect of tetracyclic amidines bearing a putrescine moiety)
RN 196296-15-8 CA
CN Benzo[k]phenanthridine-6,9-diamine, 6a,7,8,12b-tetrahydro-N9,6a,8-trimethyl-N6-pentyl-, (6aα,8β,12bα)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS

L6 ANSWER 3 OF 12 CA COPYRIGHT 2005 ACS on STN (Continued)
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L6 ANSWER 4 OF 12 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 126:330558 CA
TITLE: Preparation of aminobenzophenanthridine derivatives
INVENTOR(S): Clement, Bernd
PATENT ASSIGNEE(S): Germany
SOURCE: Ger. Offen., 5 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19538088	A1	19970417	DE 1995-19538088	19951013
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CA 2232609	AA	19970424	CA 1996-2232609	19961011
<--				
WO 9714683	A2	19970424	WO 1996-DE1958	19961011
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WO 9714683	A3	20010913		
W: AU, BG, BR, CA, CN, CZ, HU, IL, JP, KP, MX, NO, NZ, PL, RO, RU, SK, TR, UA, US, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
AU 9715895	A1	19970507	AU 1997-15895	19961011
<--				
AU 707092	B2	19990701		
EP 873315	A1	19981028	EP 1996-945501	19961011
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EP 873315	B1	20030423		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
CN 1204321	A	19990106	CN 1996-197596	19961011
JP 11515001	T2	19991221	JP 1996-515415	19961011
BR 9610971	A	19991228	BR 1996-10971	19961011
IL 123692	A1	20001121	IL 1996-123692	19961011
RU 2180333	C2	20020310	RU 1998-108615	19961011
AT 238284	E	20030515	AT 1996-945501	19961011
CZ 291821	B6	20030618	CZ 1998-1074	19961011
NO 9801655	A	19980611	NO 1998-1655	19980408
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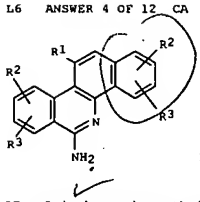
NO 313328	B1	20020916		
US 6030981	A	20000229	US 1998-51606	19980413

PRIORITY APPLN. INFO.: DE 1995-19538088 A 19951013
WO 1996-DE1958 W 19961011

OTHER SOURCE(S): MARPAT 126:330558
GI

L6 ANSWER 4 OF 12 CA COPYRIGHT 2005 ACS on STN (Continued)



I

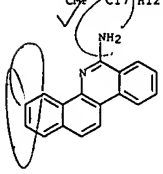
AB Aminobenzophenanthridine derivs. I [R1 = H, aryl, heteroaryl; R2, R3 = alkoxy, alkenyloxy, halogen, NO2] and their 11,12-dihydro derivs. were prepared for use as **pharmaceuticals** (no data). Thus, 2-MeC6H4CN was dimerized with CH2O in presence of Me3COK in DMPU to give 16% 6-amino-11,12-dihydrobenzo[c]phenanthridine hydrochloride which was treated with DDQ in dioxane to give 44% 6-aminobenzo[c]phenanthridine perchlorate.

IT **189577-92-2P**
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(preparation of aminobenzophenanthridine derivs.)

RN 189577-92-2 CA
CN Benzo[c]phenanthridin-6-amine, monoperchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 189577-91-1
CMF C17 H12 N2



CM 2

CRN 7601-90-3
CMF Cl H O4

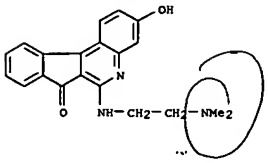
L6 ANSWER 5 OF 12 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 126:258391 CA
TITLE: Simultaneous determination of a novel anticancer **drug**, TAS-103, and its N-demethylated metabolite in monkey plasma by high-performance liquid chromatography using solid-phase extraction
AUTHOR(S): Azuma, Ryotaro; Urakawa, Akira
CORPORATE SOURCE: Pharmacokinetics Research Laboratory, Taiho Pharmaceutical Co., Ltd., 224-2, Ebisuno, Hiraishi, Kawauchi-cho, Tokushima, Japan
SOURCE: Journal of Chromatography, B: Biomedical Sciences and Applications (1997), 691(1), 179-185
CODEN: JCBBEP; ISSN: 0378-4347
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A simple and rapid method for the anal. of a novel anticancer **drug**, TAS-103, and its metabolite demethyl-TAS-103 in monkey plasma has been developed. This method is based on high-performance liquid chromatog. with visible detection at 460 nm after solid-phase extraction with a Sep-Pak Vac PS-2 cartridge. The extraction recoveries of each compound, including the internal standard TAS-1-018, were from 88 to 102. The quantitation limit of each compound was 5.0 ng/mL in 0.5 mL of plasma. The coeffs. of variation for each compound ranged from 0.9 to 4.9, and relative errors for each compound ranged from -3.8 to 4.6. Both compds. in monkey plasma were stable at -80°C for 39 days and the exts. were stable at ambient temperature for 24 h. This method has been demonstrated to be useful for the **pharmacokinetic** study of TAS-103 in monkey plasma after i.v. administration.

IT **174634-09-4**, TAS 103
RL: ANT (Analyte); BPR (Biological process); BSU (Biological study, unclassified); ANST (Analytical study); BIOL (Biological study); PROC (Process)
(determination of TAS-103 and its N-demethylated metabolite in plasma by HPLC using solid-phase extraction)

RN 174634-09-4 CA
CN 7H-Indeno[2,1-c]quinolin-7-one, 6-[[2-(dimethylamino)ethyl]amino]-3-hydroxy-, dihydrochloride (9CI) (CA INDEX NAME)

L6 ANSWER 5 OF 12 CA COPYRIGHT 2005 ACS on STN (Continued)



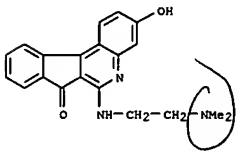
●2 HCl

L6 ANSWER 6 OF 12 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 126:258248 CA
TITLE: Theory and actual attempts to establish an effective cancer chemotherapy
AUTHOR(S): Fujimoto, Shuichi
CORPORATE SOURCE: Division of Chemotherapy, Chiba Cancer Center, Research Institute, Japan
SOURCE: Gan to Kagaku Ryoho (1997), 24(4), 501-510
CODEN: GTKRDX; ISSN: 0385-0684
PUBLISHER: Gan to Kagaku Ryohosha
DOCUMENT TYPE: Journal; General Review
LANGUAGE: Japanese

AB A review with 9 refs. To establish an effective cancer chemotherapy, theor. analyses of chemoresistance factors in recurrent patients and possible approaches to curative chemotherapy were under-taken. Multidrug resistance of tumor cells in recurrent patients may hamper the development of new antitumor agents. Thus, we developed a new screening method (FACS method) which employs fresh clin. specimens. By this method, TAS-103 was found to be far more effective than 10 standard drugs and to be one of the most effective drugs among 20 or more new antitumor agents under study. Development of several effective drugs, such as TAS-103, might lead to a curative cancer chemotherapy.

IT 174634-09-4, TAS 103
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES
(Uses)
(theory and actual attempts to establish an effective cancer chemotherapy)

RN 174634-09-4 CA
CN 7H-Indeno[2,1-c]quinolin-7-one, 6-[[2-(dimethylamino)ethyl]amino]-3-hydroxy-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

L6 ANSWER 7 OF 12 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 116:235628 CA
TITLE: Preparation of pyridines and related aza heterocycle derivatives as antihypertensives and antiarrhythmics
INVENTOR(S): Tomcufcik, Andrew Stephen; Meyer, Walter Edward; Marsico, Joseph William
PATENT ASSIGNEE(S): American Cyanamid Co., USA
SOURCE: Eur. Pat. Appl., 48 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 446604	A2	19910918	EP 1991-101496	19910205
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EP 446604	A3	19920219		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, NL, SE				
JP 04217958	A2	19920807	JP 1991-73934	19910313
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CA 2038317	AA	19910917	CA 1991-2038317	19910314
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AU 9173525	A1	19910919	AU 1991-73525	19910315
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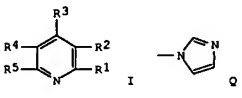
AU 640208	B2	19930819		
PRIORITY APPLN. INFO.:			US 1990-494387 A	19900316

OTHER SOURCE(S): MARPAT 116:235628
GI

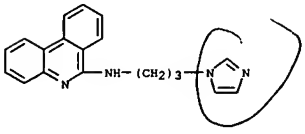


AB The title compds. [I; R1 = H, halo, NR6ZR7; R2 = H, NO2, cyano; R1R2 = CH:CHCH:CH; R3 = H, C1-3 alkyl, Ph, NR6ZR7, R2R3 = R1R2; R4 = H, NO2, cyano, C1-3 alkyl, COMe, CONH2; R3R4 = R1R2; R5 = H, halo, C1-3 alkyl, C6H4CF3-3, C6H4F-3, C6H2(OMe)3-3,4,5, pyridyl; R4R5 = R1R2, CH:C(COMe)CH:CH, NNPhN, SCH:CH, etc.; R6 = H, COMe; R7 = pyridyl, imidazolo; Z = (CH2)n; n = 1-5; with a proviso] and their pharmaceutically acceptable salts were prepared, e.g., by amination of chloropyridines with R7Z-amines. Thus, refluxing for 16 h a mixture of 31.7 g 2-chloro-3-nitropyridine and 50 g Q(CH2)3NH2 in 500 mL EtOH in the presence of EtN(CHMe2)2 gave 43.7 g title compound I [R1 = NH(CH2)3Q, R2 = NO2, R3 = R4 = R5 = H (II)] which at 1 + 10-5 M gave 80% inhibition of TXB2. II in rats at 100 mg/kg (by gavage) reduced blood pressure to 98 from 160 mmHg, and in mice at 10 mg/kg i.v. in a CaCl2- and KCl-induced arrhythmia test gave survival rate 3/6 and 4/6, resp. Approx. 69 I were prepared

L6 ANSWER 7 OF 12 CA COPYRIGHT 2005 ACS on STN (Continued)

IT 140692-33-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as antihypertensive and antiarrhythmic)

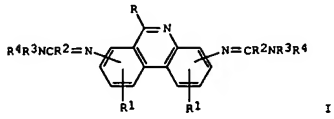
RN 140692-33-7 CA
CN 6-Phenanthridinamine, N-[3-(1H-imidazol-1-yl)propyl]- (9CI) (CA INDEX NAME)



L6 ANSWER 8 OF 12 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 103:160409 CA
TITLE: Chemotherapeutic bisamidine derivatives of substituted phenanthridines and their pharmaceutically acceptable salts
PATENT ASSIGNEE(S): Hoechst Pharmaceuticals Ltd., India
SOURCE: Indian, 26 pp.
CODEN: INXXAP
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
IN 153442	A	19840714	IN 1981-BO344	19811222
PRIORITY APPLN. INFO.:			IN 1981-BO344	19811222

GI



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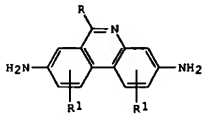
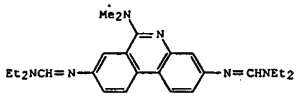


II



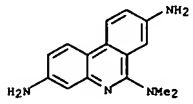
III

AB Phenanthridines I [R = H, halo, alkoxy, NH2, monoalkylamino, dialkylamino, N heterocyclyl optionally containing O, S, N; R1 = H, alkyl, alkoxy, halo, NO2, NH2; R2 = H, (un)substituted alkyl; R3, R4 = H, alkyl; C(R2)R3N = heterocyclyl; NR3R4 = heterocyclyl] were prepd. by treating diaminophenanthridines II with R2CONR3R4 and POCl3. Thus, 3,8-diamino-6-dimethylaminophenanthridine was added to a mixt. of Et2NCHO and POCl3 to give 71% phenanthridine III. I are useful as amebicides and protozoacides (no data).

L6 ANSWER 8 OF 12 CA COPYRIGHT 2005 ACS on STN (Continued)

IT 93494-47-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with diethylformamide)

RN 93494-47-4 CA
CN 3,6,8-Phenanthridinetriamine, N6,N6-dimethyl- (9CI) (CA INDEX NAME)



L6 ANSWER 9 OF 12 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 81:13559 CA
TITLE: Benzazine derivatives
INVENTOR(S): Rodway, Ronald E.; Cookson, Ronald F.
PATENT ASSIGNEE(S): Aspro-Nicholas Ltd.
SOURCE: S. African, 138 pp.
CODEN: SFXXAB
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

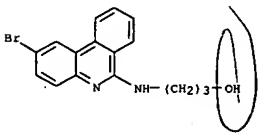
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
ZA 7201118	A	19731031	ZA 1972-1118	19720221
PRIORITY APPLN. INFO.:			ZA 1972-1118 A	19720221

GI For diagram(s), see printed CA Issue.

AB Benzazine compds. I-VII [X = CH2CH2, CH : CH, (CH2)3, R, R1 = H, Ph, substituted Ph, NO2, halo] with analgesic, antiinflammatory, antibacterial, antiviral and cardiovascular activity were prepared Thus, a mixture of phenyl phthalazone and ethylene-diamine monotosylate was heated at 240° for 20 hr, extracted with hot dilute HCl and then basicified with NaOH to give II (X = CH2CH2, R = Ph).

IT 38052-92-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 38052-92-5 CA
CN 1-Propanol, 3-[(2-bromo-6-phenanthridinyl)amino]- (9CI) (CA INDEX NAME)

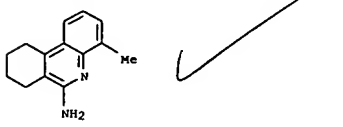


L6 ANSWER 10 OF 12 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 43:8385 CA
ORIGINAL REFERENCE NO.: 43:1778g-i,1779a-e
TITLE: New syntheses of heterocyclic compounds. IX. Tetrahydrophenanthridines
AUTHOR(S): Hollingsworth, B. L.; Petrow, V.
SOURCE: Journal of the Chemical Society, Abstracts (1948) 1537-41
CODEN: JCSAAZ; ISSN: 0590-9791
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 43:8385

GI For diagram(s), see printed CA Issue.

AB cf. C.A. 41, 967i. Work on the relationship between structure and analeptic activity has been extended by the preparation of some 9-amino- and tetrahydro-9-aminophenanthridines (I, R = NH2) by direct amination of the corresponding bases (the pharmacol. data will be published by Thorp). Cyclohexanone (50 g.), 9 g. (HCHO)3, and 11 g. Et2NH.HCl, heated until the Mannich base is formed, treated with 9.3 g. PhNH2, 12.8 g. PhNH2.HCl, and 13 g. SnCl4.5H2O and refluxed 16 h., give 45% 5,6,7,8-tetrahydrophenanthridine (Ia) (I, R = H), m. 63° (C.A. 31, 7061.9); omission of SnCl4 reduced the yield to 15% and of PhNH2.HCl to less than 5%. o-MeC6H4NH2 gives 40% of the 1-Me derivative of Ia and p-MeC6H4NH2 gives 50% of the 3-Me derivative m-MeC6H4NH2 gives 15% of the 2(or 4)-Me derivative, b20 210° [picrate, yellow, m. 226° (decomposition)]. 5-Methyl-1-(diethylaminomethyl)-2-cyclohexanone and PhNH2 give 12% of the 7-Me derivative of Ia. 3,5-Me2C6H3NH2-gives 20% of the 1,3-di-Me derivative of Ia and 2,5-Me2C6H3NH2 gives 20% of the 1,4-isomer. o-MeOC6H4NH2 gives 25% of the 1-MeO derivative of Ia, yellow, m. 106° [picrate, mustard-yellow, m. 214° (decomposition)]; p-MeOC6H4NH2 gives 50% of the 3-MeO isomer. p-O2NC6H4NH2 yields 50% of the 3-NO2 derivative of Ia, m. 172-3° [picrate, m. 203° (decomposition)]. p-ClC6H4NH2 gives 30% of the 3-Cl derivative of Ia. p-PhC6H4NH2 yields 40% of the 3-Ph derivative of Ia, m. 122-3° [picrate, yellow, m. 235° (decomposition)]. 1-(1-Naphthyliminomethyl)-2-cyclohexanone (II) (50 g.) and 400 mL. anhydrous HCO2H, refluxed 20 h., give 60% 5,6,7,8-tetrahydro-1,2-benzophenanthridine and the 2-naphthyl isomer of II gives 75% of the 3,4-isomer. 5-Aminoacenaphthene and formylcyclohexanone give 1-(5-acenaphthenyliminomethyl)-2-cyclohexanone, orange-yellow, m. 137-8°; this yields 50% 1,2,3,4-tetrahydro-11-aza-6,7-acechrysene (III), cream, m. 134-5° [picrate, yellow, m. 252-3° (decomposition)]. Ia (5 g.), 25 g. PhNEt2, and 6 g. NaNH2, heated 5 h. at 170°, give 4 g. of the 9-NH2 derivative (IV), m. 165°; acetate, prepared in excess hot AcOH, m. 212-13°. IV (5 g.) in 300 mL. dilute HCl, treated with 4 g. NaNO2 in 40 mL. ice-cold H2O and heated 1 h. on the water bath, gives 4 g. 5,6,7,8-tetrahydrophenanthridone, m. 272°. 9-Amino-1-methyl-5,6,7,8-tetrahydrophenanthridine, m. 121-2°, 45%; 3-Me isomer, m. 169-70°, 90% (acetate m. 204-5°); 1,3-di-Me derivative, m. 136-7°, 60%. 9-Amino-5,6,7,8-tetrahydro-3,4-benzophenanthridine, m. 241-2°, 80%. The 1-Me derivative of Ia (10 g.) and 10 g. Se, heated 5 h. at 300°, give 85% 1-methylphenanthridine,

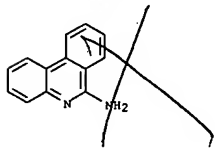
L6 ANSWER 10 OF 12 CA COPYRIGHT 2005 ACS on STN (Continued)
m. 95°; 7 g., 25 mL. PhNEt2, and 8 g. NaNH2, heated 4 h. at 160°, give 50% of the 9-NH2 deriv., m. 116-17°. 9-Amino-3-methylphenanthridine, m. 170-1°, 60%; the 1,3-di-Me compd. m. 142-3°, 55%.
IT 855623-05-1, Phenanthridine, 6-amino-7,8,9,10-tetrahydro-4-methyl- (preparation of)
RN 855623-05-1 CA
CN Phenanthridine, 6-amino-7,8,9,10-tetrahydro-4-methyl- (5CI) (CA INDEX NAME)



L6 ANSWER 11 OF 12 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 33:22099 CA
ORIGINAL REFERENCE NO.: 33:3173a-d
TITLE: Picrylamino compounds; diazalines
INVENTOR(S): Morgan, Gilbert T.; Stewart, Jessie
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

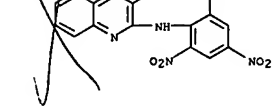
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 496258		19381128	GB	

<--
AB Picrylamino, compds. are prepared by condensing picryl chloride (I) or an alkyl derivative thereof, e. g., methyl- and dimethyl-picryl chlorides, with a compound containing a tertiary cyclic N atom and an adjacent amino group, e. g., 2-aminopyridine (II), 2-aminoquinoline, 1-aminoisoquinoline, 9-aminophenanthridine and their homologs. By cautious heating, preferably in the presence of PhOH, dimethylaniline, etc., ring closure takes place with formation of dinitro-1,3-diazalines, from which 1,3-diazalines may be obtained by reduction and elimination of the amino groups formed. The products are useful as intermediates for the manufacture of dyes and drugs. Among examples, (1) I is heated in C6H6 solution with II to give N-picryl-2-aminopyridine; when PhMe is used as solvent, ring closure takes place with formation of 1,2-pyrido-7,9-dinitro-4,5-benzo-1,3-diazaline, (2) by heating the diazaline of (1) with an aqueous solution of Na polysulfide, 1,2-pyrido-7,9- or -9,7-nitroamino-4,5-benzo-1,3-diazaline is produced; when H is used as reducing agent under an initial pressure of 5 atmospheric and in the presence of Pt oxide, 1,2-pyrido-7,9-diamino-4,5-benzo-1,3-diazaline (III) is produced while at H pressures maintained at 8-10 atmospheric tetrahydro-III results.
IT 832-68-8, Phenanthridine, 6-amino- (ring closure of derivs. of)
RN 832-68-8 CA
CN 6-Phenanthridinamine (9CI) (CA INDEX NAME)



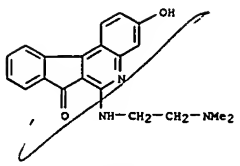
L6 ANSWER 12 OF 12 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 33:3973 CA
ORIGINAL REFERENCE NO.: 33:594i,595a-i,596a-d
TITLE: Pyrido(1',2',1,2)benziminazoles and allied compounds (cyclic 1,3-diazalines)
AUTHOR(S): Morgan, Gilbert T.; Stewart, Jessie
SOURCE: Journal of the Chemical Society, Abstracts (1938) 1292-305
CODEN: JCSAAZ; ISSN: 0590-9791
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
GI For diagram(s), see printed CA Issue.
AB The α-NH2 derivs. of pyridine, quinoline and isoquinoline readily obtainable from these bases by the NaNH2 condensation are favorable starting materials in the preparation of substances having a pyridinic or quinolinic structure likely to be of interest as either color intermediates or therapeutic agents. 5-Amino-2,2'-dipyridylamine (I), m. 91°, results from catalytic reduction of the 5-NO2 derivative in absolute EtOH at 50°. 2-Aminopyridine (II) and 2,4-(O2N)2C6H3Cl, heated at 120° for 2 hrs., give N,2',4'-dinitrophenyl-2-aminopyridine (III), golden needles, m. 156-7°; I gives N,2'',4''-dinitrophenyl-5-amino-2,2'-dipyridylamine (IV), red, m. 198°; these 2 NO2 derivs. possess tinctorial properties toward acetate rayon similar to the Dispersol yellows. Catalytic reduction of III gives the di-NH2 derivative, m. 150°; the di-NH2 derivative from IV m. 187°. II and picryl chloride, refluxed in C6H6 for 1 hr., give N,2',4',6'-trinitrophenyl-2-aminopyridine (V), m. 135°; I gives N,2'',4'',6''-trinitrophenyl-5-amino-2,2'-dipyridylamine, ruby-red, m. 224°. V forms a N-Me derivative, bright red, m. 243°. V may be represented in 2 tautomeric forms on the supposition that the H atom of the picramido group migrates to the adjacent N atom of the C5H5N ring; in 1 case, on loss of HNO2, a dinitro-α-carboline would result, in the other a di-NO2 derivative of a new hydroaromatic base (VI), designated pyrido-(1',2',1,2)benziminazole (numbering as in VII) or 1,2-pyrido-4,5-benzo-1,3-diazaline (numbering as in VIII). Refluxing V in PhNMe2 for 2-2.5 hrs. gives the 4,6-di-NO2 derivative (IX) of VI, bright yellow, m. above 300°; PhNMe2. in PhNO2, PhOH in PhNO2 or PhOH alone also give IX; V also gives IX on heating at 135° until frothing ceases and then at 200-20°; IX also results when V is prepared in PhMe in place of C6H6. Catalytic reduction of IX gives the 4,6-di-NH2 derivative (X), yellow, m. 204-5°, while Na2S in 50% aqueous Me2CO gives the 4,6(or 6,4)-nitroamino derivative of VI, dark red, m. above 280°. Removal of the NH2 group by reduction of the diazo compound with 50% EtOH gives the 4(or 6)-NO2 derivative of VI, bright yellow, m. 260-2°; catalytic reduction gives the 4(or 6)-NH2 derivative (XI), yellow, m. 229-30°. Removal of the NH2 group from XI or the 2 NH2 groups from X gives VI, m. 178-9°; it has an aniseed-like odor, while the isomeric α-carboline (XII) is odorless; unlike XII, VI does not exhibit pronounced blue fluorescence in neutral solvents nor does it develop on reduction the characteristic deep blue color with p-Me2NC6H4CHO. Catalytic reduction of VI in EtOH at 50° (PtO2 at 10-8 atmospheric) gives the 3',4',5',6'-tetrahydro derivative of X, m. 201-2°; a higher H2 pressure or a higher temperature did not cause further reduction; through the diazo reaction this yields the 3',4',5',6'-tetrahydro derivative

L6 ANSWER 12 OF 12 CA COPYRIGHT 2005 ACS on STN (Continued)
of VI, m. 107°. The diazo compd. from VIII with NaN3 gives 4,6-bistriazopyrido(1',2',1,2)benziminazole, C11H6N8, decomps. 167-70°; the 3',4',5',6'-tetrahydro deriv. m. 132°. 2-Amino-3-methylpyridine and picryl chloride in C6H6 give N-picryl-2-amino-3-methylpyridine, yellow, m. 142-3°; PhOH in xylene gives 4,6-dinitro-3'-methylpyrido(1',2',1,2)benziminazole (XIII), yellow, m. 256-60°; catalytic reduction of XIII gives the di-NH2 deriv., yellow, m. about 130°; Na2S and S in dil. aq. Me2CO reduce XIII to the 4,6(or 6,4)-nitroamino deriv., red, m. 269-70°; removal of the NH2 group gives the 4(or 6)-NO2 deriv., yellow, m. 260-2° and reduced catalytically to the 4(or 6)-NH2 deriv., m. 185-7°; removal of this NH2 group gives 3'-methylpyrido(1',2',1,2)benziminazole, m. 162°. 2-Aminoquinoline yields a picryl deriv., yellow, m. above 280°; heating with an equal wt. of PhOH in xylene gives 4,6-dinitroquinolo(1',2',1,2)benziminazole, yellow, m. above 300°; the 4,6-di-NH2 deriv., yellow, m. 273-4°, results in 75% yield on catalytic reduction in abs. EtOH at an initial pressure of 31 atm. The 4,6(or 6,4)-nitroamino deriv., brick-red, m. above 300°; the 4(or 6)-NO2 deriv., yellow, m. 242-3°; this gives the yellow-green 4(or 6)-NH2 deriv., m. 223°. Quinolo(1',2',1,2)benziminazole, m. 102°, results from either the mono- or di-NH2 deriv. 1-Aminoisoquinoline yields a red picryl deriv., m. 156°; PhOH in xylene gives 4,6-dinitroisoquinolo-(2',1',1,2)benziminazole, golden needles, m. above 280°; the 4,6-di-NH2 deriv. m. 249-50°; reduction of the diazo compd. with abs. EtOH gives isoquinolo(2',1',1,2)-benziminazole, m. 129° which becomes a pale pink-buff on exposure to light and air. 9-Aminophenanthridine reacts with picryl chloride only in boiling xylene and the resulting picryl deriv. is contaminated with XIV; the pure deep yellow infusible deriv. could be obtained by using small quantities of the reactants. Boiling the mixt. with PhNMe2 gives 4,6-dinitrophenanthrido (10',9',1,2) benziminazole (XIV), deep yellow, m. above 280°; 4,6-di-NH2 deriv., yellow, the reduction being carried out at 80-90° with an initial H pressure of 31 atm.; removal of the NH2 groups gives phenanthrido(10',9',1,2)benziminazole, m. 153-4°.
IT 861002-25-7, Phenanthridine, 6-(2,4,6-trinitroanilino)- (preparation of)
RN 861002-25-7 CA
CN Phenanthridine, 6-(2,4,6-trinitroanilino)- (4CI) (CA INDEX NAME)



L8 ANSWER 1 OF 77 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 128:43507 CA
TITLE: Antitumor activity of a novel quinoline derivative, TAS-103, with inhibitory effects on topoisomerases I and II
AUTHOR(S): Utsugi, Teruhiro; Aoyagi, Kumio; Asao, Tetsuji; Okazaki, Shinji; Aoyagi, Yoshimi; Sano, Masaki; Wierzba, Konstanty; Yamada, Yuji
CORPORATE SOURCE: Hanno Research Center, Taiho Pharmaceutical Co., Ltd., Hanno, 357, Japan
SOURCE: Japanese Journal of Cancer Research (1997), 88(10), 992-1002
CODEN: JJCREP; ISSN: 0910-5050
PUBLISHER: Japanese Cancer Association
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A novel quinoline derivative, TAS-103 (6-[[2-(dimethylamino)ethyl]amino]-3-hydroxy-7H-indeno[2,1-c]quinolin-7-one dihydrochloride), was developed as an anticancer agent targeting topoisomerases (topo) I and II, with marked efficacy in solid tumors. TAS-103 inhibited topo I and II (IC50: 2 μM, 6.5 μM) at a concentration similar to or lower than those of previous agents, and had a strong cytotoxic effect on P388 and KB cells (IC50: 0.0011 μM, 0.0096 μM). TAS-103 stabilized top I and II-DNA complex to that induced by etoposide (VP-16) but a smaller amount of topo I-DNA complex than that produced by camptothecin (CPT). In the in vivo study, intermittent i.v. administration was markedly effective against s.c.-implanted murine tumors. Furthermore, TAS-103 had marked efficacy against various lung metastatic tumors, and a broad antitumor spectrum in human tumor xenografts (derived from lung, colon, stomach, breast, and pancreatic cancer). The efficacy of TAS-103 was generally greater than that of irinotecan (CP-11), VP-16, or cis-diamminedichloroplatinum (CDDP).
IT 174634-09-4, TAS-103
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(antitumor activity of TAS-103 and inhibitory effects on topoisomerases I and II)
RN 174634-09-4 CA
CN 7H-Indeno[2,1-c]quinolin-7-one, 6-[[2-(dimethylamino)ethyl]amino]-3-hydroxy-, dihydrochloride (9CI) (CA INDEX NAME)

L8 ANSWER 1 OF 77 CA COPYRIGHT 2005 ACS on STN (Continued)



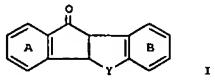
●2 HCl

REFERENCE COUNT: 42 THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

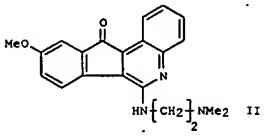
L8 ANSWER 2 OF 77 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 127:81361 CA
TITLE: Preparation of indenoquinoline derivatives and analogs as antitumor agents
INVENTOR(S): Asao, Tetsuji; Okazaki, Shinji; Wakita, Sukeji; Utsuki, Teruhiro; Yamada, Yuji
PATENT ASSIGNEE(S): Taiho Pharmaceutical Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 12 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 09143166 <--	A2	19970603	JP 1995-299420	19951117
JP 3643916	B2	20050427		
PRIORITY APPLN. INFO.:			JP 1995-299420	19951117

OTHER SOURCE(S): MARPAT 127:81361
GI



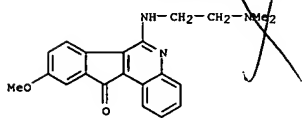
I



II

AB The title compds. I [ring A, B = benzene ring which may have substituents such as halo, alkoxy, etc.; Y = R1C:N, etc.; R1 = NR3R4, etc.; R3, R4 = H, Ph, etc.] are prepared The title compound II.2HCl at 225 mg/kg/day for 2 days gave 35% increase in the survival time of mice with transplanted P388 leukemic cells.
IT 191801-82-8P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of indenoquinoline derivs. and analogs as antitumor

L8 ANSWER 2 OF 77 CA COPYRIGHT 2005 ACS on STN (Continued)
RN 191801-82-8 CA
CN 11H-Indeno[1,2-c]quinolin-11-one, 6-[[2-(dimethylamino)ethyl]amino]-9-methoxy-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

L8 ANSWER 3 OF 77 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 124:232268 CA
TITLE: Preparation and formulation of indenoquinolines as antitumor agents
INVENTOR(S): Okazaki, Shinji; Asao, Tetsuji; Wakida, Motoji; Ishida, Keisuke; Washinosu, Masato; Utsugi, Teruhiro; Yamada, Yuji
PATENT ASSIGNEE(S): Taiho Pharmaceutical Co., Ltd., Japan
SOURCE: PCT Int. Appl., 146 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9532187	A1	19951130	WO 1995-JP944	19950518
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RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
TW 440562	B	20010616	TW 1995-84104882	19950517
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CN 1130903	A	19960911	CN 1995-190639	19950518
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CN 1131216	B	20031217		
HU 75651	A2	19970528	HU 1996-130	19950518
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HU 218308	B	20000728		
JP 2840796	B2	19981224	JP 1995-530192	19950518
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RU 2124017	C1	19981227	RU 1996-105034	19950518
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CA 2167382	C	19990831	CA 1995-2167382	19950518
IL 113778	A1	19990922	IL 1995-113778	19950518
AT 203236	E	20010815	AT 1995-918733	19950518
ES 2158109	T3	20010901	ES 1995-918733	19950518
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US 5733918	A	19980331	US 1996-578542	19960119
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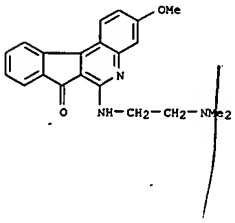
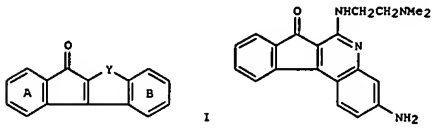
L8 ANSWER 3 OF 77 CA COPYRIGHT 2005 ACS on STN (Continued)



L8 ANSWER 3 OF 77 CA COPYRIGHT 2005 ACS on STN (Continued)

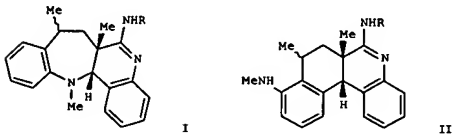
US 6028079	A	20000222	US 1997-909934	19970812
GR 3036795	T3	20020131	GR 2001-401657	20011004
PRIORITY APPLN. INFO.:			JP 1994-107190	A 19940520
			WO 1995-JP944	W 19950518
			US 1996-578542	A3 19960119

OTHER SOURCE(S): MARPAT 124:232268
GI



AB The title compds. I [ring A represents an optionally substituted benzene or naphththalene ring, or a benzene ring having an lower alkylenedioxy group; ring B represents a benzene ring which may be substituted or has a lower alkylenedioxy group; Y represents N:CR or CR(:N); R represents NR1R2, OR3 or an optionally substituted nitrogenous heterocyclic group; R1 and R2 are the same or different from each other and each represents hydrogen, Ph, an optionally substituted nitrogenous heterocyclic group, or a lower alkyl group which may be substituted by at least one substituent selected from the group consisting of optionally substituted amino, lower alkoxy, Ph, a nitrogenous heterocyclic group, an amine oxide group substituted by lower alkyl, and hydroxy; and R3 represents lower alkyl which may be substituted by substituted amino, provided the case where R represents an optionally substituted nitrogenous heterocyclic group and rings A and B represent each an unsubstituted benzene ring, is excluded] are prepared The title compound II.3HCl (preparation given) in vitro showed IC50 of 1.1 x 10-2 μg/mL against p388 mouse leukemic cells.
IT 174634-05-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of indenoquinolines as antitumor agents)
RN 174634-05-0 CA
CN 7H-Indeno[2,1-c]quinolin-7-one, 6-[[2-(dimethylamino)ethyl]amino]-3-methoxy- (9CI) (CA INDEX NAME)

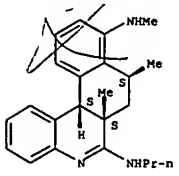
L8 ANSWER 4 OF 77 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 124:202063 CA
TITLE: Relationship between cytotoxicity and DNA-binding affinity of amidine derivatives of tetrahydroquino[4,3-b][1]benzazepines and tetrahydrobenzo[k]naphthyridines
AUTHOR(S): Eifler-Lima, V. L.; Uriac, P.; Huet, J.; Jenkins, T. C.; Thurston, D. E.
CORPORATE SOURCE: Lab. Chim. Pharmaceutique, Fac. Pharmacie, Rennes, 35043, Fr.
SOURCE: Bioorganic & Medicinal Chemistry Letters (1995), 5(24), 3003-6
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



AB Amidines I and II [R = Pr, (CH2)3OH, (CH2)3NH2, (CH2)4NH2] have been synthesized. All the compds. showed weak but significant DNA-binding affinity which correlated with in vitro cytotoxicity across two cell lines.
IT 173960-71-9P
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process)
(preparation, DNA binding, and cytotoxicity of aminoquinobenzazepines and aminobenzonaphthyridines)
RN 173960-71-9 CA
CN Benzo[k]phenanthridine-6,9-diamine, 6a,7,8,12b-tetrahydro-N9,6a,8-trimethyl-N6-propyl-, dihydrochloride, (6aα,8α,12bα)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L8 ANSWER 4 OF 77 CA COPYRIGHT 2005 ACS on STN (Continued)



●2 HCl

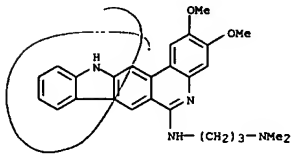
L8 ANSWER 5 OF 77 CA COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 123:32984 CA
TITLE: A Versatile Construction of the 8H-Quino[4,3-b]carbazole Ring System as a Potential DNA Binder
AUTHOR(S): Mohanakrishnan, Arasambattu K.; Srinivasan, Panayencheri C.
CORPORATE SOURCE: Department of Organic Chemistry, University of Madras, Madras, 600 025, India
SOURCE: Journal of Organic Chemistry (1995), 60(7), 1939-46
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A short synthesis of quino[4,3-b]- and quino[3,4-b]carbazoles is reported.
The key step involves the preparation of suitable 2,3-divinylindoles by consecutive Wittig reactions. The thermal electrocyclic reaction of the divinylindole, with concomitant dehydrogenation in the presence of Pd-C, gave the (nitroaryl)carbazole, which, on reductive cyclization, led to the quinocarbazole. Cleavage of the phenylsulfonyl group, followed by phosphorus oxychloride treatment and subsequent displacement of the chlorine with 3-(dimethylamino)propylamine, gave the title compds. in 25-30% overall yield.

IT 164261-69-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of quinocarbazole ring systems)

RN 164261-69-2 CA
CN 1,3-Propanediamine, N'-(2,3-dimethoxy-5,12-dihydro-12H-indolo[3,2-j]phenanthridin-6-yl)-N,N-dimethyl- (9CI) (CA INDEX NAME)



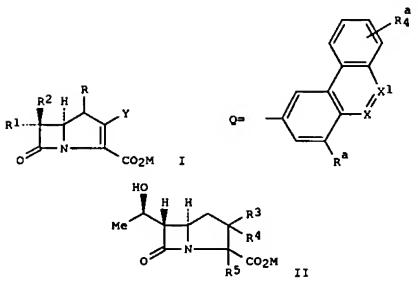
L8 ANSWER 6 OF 77 CA COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 122:187249 CA
TITLE: Preparation of 2-phenanthridinylcarbapenems as antibacterial agents
INVENTOR(S): Dininno, Frank P.; Greenlee, Mark L.; Rano, Thomas A.; Lee, Wendy
PATENT ASSIGNEE(S): Merck and Co., Inc., USA
SOURCE: PCT Int. Appl., 115 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9417066	A1	19940804	WO 1994-US85	19940103
W: AU, BB, BG, BR, BY, CA, CN, CZ, FI, HU, JP, KR, KZ, LK, LV, MG, MN, MW, NO, NZ, PL, RO, RU, SD, SK, UA, US, UZ				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
US 5336674	A	19940809	US 1993-9626	19930127
CA 2154276	AA	19940804	CA 1994-2154276	19940103
AU 9459902	A1	19940815	AU 1994-59902	19940103
EP 682666	A1	19951122	EP 1994-906014	19940103
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
JP 08505874	T2	19960625	JP 1994-517039	19940103
PRIORITY APPLN. INFO.:			US 1993-9626 A	19930127
			WO 1994-US85 W	19940103

OTHER SOURCE(S): MARPAT 122:187249
GI

L8 ANSWER 6 OF 77 CA COPYRIGHT 2005 ACS on STN (Continued)



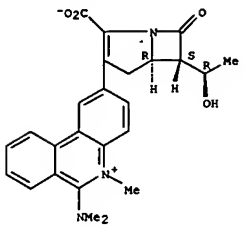
AB Title compds. [I; M = H, alkali metal, neg. charge, etc.; .; R = H, Me; R1,R2 = H, Me, Et, CH2OH, MeCH(OH), etc.; .; Y = phenanthridinyl group Q; 1 of Ra = H and the others = H, CF3, halo, (un)substituted alkoxy; 1 of X,X1 = N+Rdm and the other = CRc; Rc = H, (un)substituted alkyl(oxy), NH2, etc.; .; Rd = H, NH2, O-, alkyl, etc.; .; m = 0 or 1] were prepared as antibacterial agents (no data). Thus, oxopenamcarboxylate II [M = CH2C6H4(NO2)-4; R3R4 = O, R5 = H] was condensed with Me3SnQ CF3SO3- (Ra = H, X = N+Me, X1 = CH) and the product hydrogenolized to give II (M = neg. charge, R3 = Q, R4R5 = bond, Ra = H, X = N+Me, X1 = CH).

IT 161546-79-8P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of phenanthridinylcarbapenems as antibacterial agents)

RN 161546-79-8 CA
CN Phenanthridinium, 2-[2-carboxy-6-(1-hydroxyethyl)-7-oxo-1-azabicyclo[3.2.0]hept-2-en-3-yl]-6-(dimethylamino)-5-methyl-, inner salt, [5R-[5α,6α(R*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L8 ANSWER 6 OF 77 CA COPYRIGHT 2005 ACS on STN (Continued)



L8 ANSWER 7 OF 77 CA COPYRIGHT 2005 ACS on STN

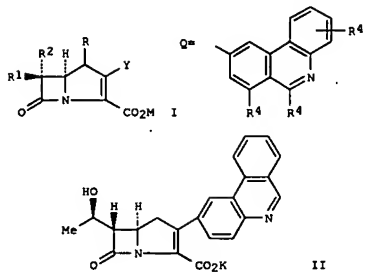
ACCESSION NUMBER: 122:187248 CA
TITLE: 2-(phenanthridinyl)carbapenem antibacterial agents
INVENTOR(S): Dininno, Frank P.; Greenlee, Mark L.; Rano, Thomas A.; Lee, Wendy
PATENT ASSIGNEE(S): Merck and Co., Inc., USA
SOURCE: U.S., 28 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5328904	A	19940712	US 1993-9622	19930127
CA 2154275	AA	19940804	CA 1994-2154275	19940103
WO 9417065	A1	19940804	WO 1994-US62	19940103
W: AU, BB, BG, BR, BY, CA, CN, CZ, FI, HU, JP, KR, KZ, LK, LV, MG, MN, MW, NO, NZ, PL, RO, RU, SD, SK, UA, US, UZ				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9461207	A1	19940815	AU 1994-61207	19940103
EP 682667	A1	19951122	EP 1994-907775	19940103
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
JP 08505873	T2	19960625	JP 1994-517034	19940103

PRIORITY APPLN. INFO.: US 1993-9622 A 19930127
WO 1994-US62 W 19940103

OTHER SOURCE(S): MARPAT 122:187248
GI

L8 ANSWER 7 OF 77 CA COPYRIGHT 2005 ACS on STN (Continued)

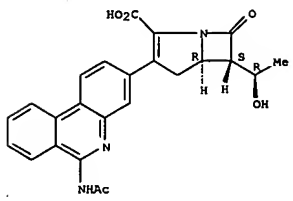


AB The title compds. [I; M = H, carboxyl-protecting group, alkali metal; R = H, Me; R1, R2 = H, Me, Et, Me2CH, HOCH2, etc.; Y = Q, (un)substituted phenanthridinyl, etc.; R4 = H, CF3, halogen, C1-4 alkoxy], useful as antibiotics (no data), are prepared Thus, carbapenem II was prepared from 2-bromophenanthridine in 3 steps.

IT 161667-42-1
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(preparation of 2-(phenanthridinyl)carbapenem antibacterial agents)

RN 161667-42-1 CA
CN 1-Azabicyclo[3.2.0]hept-2-ene-2-carboxylic acid, 3-[6-(acetylamino)-3-phenanthridinyl]-6-(1-hydroxyethyl)-7-oxo-, monosodium salt, [5R-[5α,6α(R*)]]- (9CI) (CA INDEX NAME)

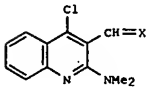
Absolute stereochemistry.

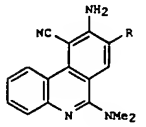


● Na

L8 ANSWER 7 OF 77 CA COPYRIGHT 2005 ACS on STN (Continued)

L8 ANSWER 8 OF 77 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 121:300738 CA
TITLE: Reactions of 2-(dimethylamino)-3-formyl-4-chloroquinoline with cyanoacetic acid derivatives
AUTHOR(S): Nesterova, I. N.; Alekseyeva, L. M.; Granik, V. G.
CORPORATE SOURCE: VNIIHhFI, Moscow, Russia
SOURCE: Khimiko-Farmatsevticheskii Zhurnal (1993), 27(1), 71-5
CODEN: KHFZAN; ISSN: 0023-1134
DOCUMENT TYPE: Journal
LANGUAGE: Russian
GI


I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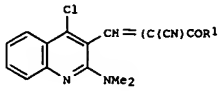
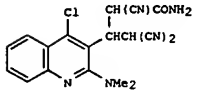

III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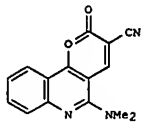
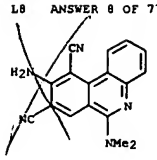
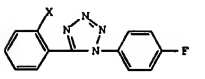

V

AB The conversion of quinoline derivative I (X = O) to compds. such as I [X = C(CN)2], II (R = CN, CO2Et), III (R1 = NH2, OEt), IV, and V is reported.
IT 159112-49-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 159112-49-9 CA
CN 8,10-Phenanthridinedicarbonitrile, 9-amino-6-(dimethylamino)- (9CI) (CA INDEX NAME)

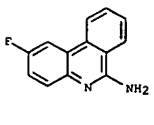
L8 ANSWER 8 OF 77 CA COPYRIGHT 2005 ACS on STN (Continued)



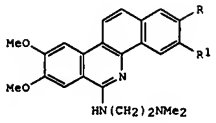
L8 ANSWER 9 OF 77 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 120:323392 CA
TITLE: Cyclizations. Part 1. Electrochemical and photochemical reactions of 1-(4-fluorophenyl)-5-(2-halogenophenyl)tetrazoles
AUTHOR(S): Donnelly, Shileen; Grimshaw, James; Trocha-Grimshaw, Jadwiga
CORPORATE SOURCE: Sch. Chem., Queen's Univ., Belfast, BT9 5AG, UK
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1993), (14), 1557-62
CODEN: JCPRB4; ISSN: 0300-922X
DOCUMENT TYPE: Journal
LANGUAGE: English
GI


I

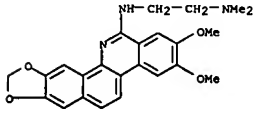
AB Electrochem. reduction of the title compds. I (R = Cl, Br, I) leads to cleavage of the carbon-halogen bond to leave a Ph radical. Competition then follows between intramol. radical substitution giving 7-fluorotetrazolo[1,5-f]phenanthridine and further reduction of the radical, then protonation, giving 1-(4-fluorophenyl)-5-phenyltetrazole. Substitution predominates but reduction and protonation becomes a more competing reaction when X = Br, I. Photochem. reaction of I confirms competition between C-X bond cleavage to give 7-fluoroetrazolo[1,5-f]phenanthridine and loss of nitrogen followed by cyclization to give 2-halophenyl-5-fluorobenzimidazole. C-X bond cleavage predominates and becomes the only reaction when the X = I. The fluorine substituent permits determination of product yields by 19F NMR spectroscopy.
IT 153386-16-4P
RL: PREP (Preparation)
(formation in electrochem. reduction of fluorotetrazolophenanthridine)
RN 153386-16-4 CA
CN 6-Phenanthridinamine, 2-fluoro- (9CI) (CA INDEX NAME)



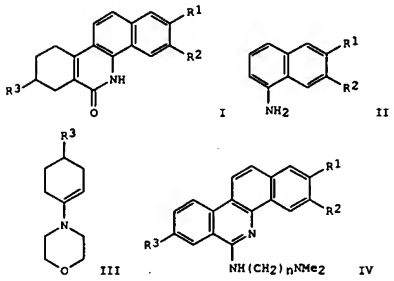
L8 ANSWER 10 OF 77 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 120:270904 CA
TITLE: A formal new access to the benzo[c]phenanthridine alkaloids, synthesis of nitidine and O-methyl fagaronine analog
AUTHOR(S): Janin, Yves L.; Bisagni, Emile
CORPORATE SOURCE: Sect. Biol., Inst. Curie, Orsay, 91405, Fr.
SOURCE: Tetrahedron (1993), 49(45), 10305-16
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 120:270904
GI


I

AB Previously unreported 2-aryl-1-naphthylamines were obtained in good yields from 2-aryl-1-tetralone oximes by using the Semmler-Wolf reaction but omitting the acetic anhydride usually present in the reaction mixture From these amines, through the thermal cyclization of their corresponding Et carbamates, a new access to the benzo[c]phenanthridin-6(5H)-ones was found. Preparation of water-soluble nitidine and O-Me fagaronine analogs bearing an alkylamino side chain on the C-6 position I (RR1 = OCH2O; R = R1 = MeO) was achieved from these compds.
IT 154283-53-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 154283-53-1 CA
CN 1,2-Ethanediamine, N'-(2,3-dimethoxy[1,3]benzodioxolo[5,6-c]phenanthridin-13-yl)-N,N-dimethyl- (9CI) (CA INDEX NAME)

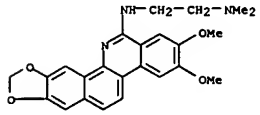


L8 ANSWER 11 OF 77 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 120:270049 CA
TITLE: Synthesis and evaluation of new 6-amino- substituted benzo[c]phenanthridine derivatives
AUTHOR(S): Janin, Yves L.; Croisy, Alain; Riou, Jean Francois; Bisagni, Emile
CORPORATE SOURCE: Sect. Biol. Inst. Curie, Inst. Curie, Orsay, F-91405, Fr.
SOURCE: Journal of Medicinal Chemistry (1993), 36(23), 3686-92
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 120:270049
GI

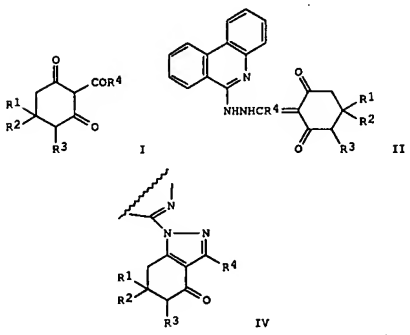


AB 7,8,9,10-Tetrahydrobenzo[c]phenanthridin-6(5H)-ones I (R1-R3 = H; R1 = R3 = OMe, R2 = H; R1 = R3 = H, R2 = OMe; R1 = OMe, R2 = R3 = H; R1 = OCHMe2, R2 = H, R3 = OMe) were prepared by using a one-pot procedure which includes the preparation of various 6- and 7-alkoxy-1-naphthyl isocyanates from 1-naphthylamines II and triphosgene, followed by addition of 1-morpholino-1-cyclohexenes III, and cyclization of the resulting amides upon heating in the presence of hydrogen chloride. Subsequent aromatization, chlorination, and substitution with (dimethylamino)alkylamines, followed by a demethylation or a selective desisopropylation, allowed synthesis of benzo[c]phenanthridine derivs. IV (R1 = H, OMe, OCHMe2, OH; R2 = H, OMe, OH; R3 = H, OMe, OH: n = 2, 3) bearing a [(dimethylamino)alkyl]amino side chain at their 6-position. These compds. were devised to further study the structure-activity

L8 ANSWER 11 OF 77 CA COPYRIGHT 2005 ACS on STN (Continued)
relationships in the benzo[c]phenanthridine family of antitumor alkaloids led by fagaronine and nitidine. Topoisomerases I and II cleavable complex assay and evaluation of the cytotoxicity and antitumor properties were performed. In vitro cytotoxicity (L1210 and Calc 18) shows a relationship between the cytotoxicity of these compds. and their topoisomerase poisoning properties. However, all these compds. were devoid of significant antitumor effect on the P388 murine leukemia system.
IT 154283-53-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(cytotoxicity and topoisomerase-inhibiting activity of)
RN 154283-53-1 CA
CN 1,2-Ethanediamine, N'-(2,3-dimethoxy[1,3]benzodioxolo[5,6-c]phenanthridin-13-yl)-N,N-dimethyl- (9CI) (CA INDEX NAME)

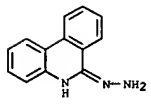


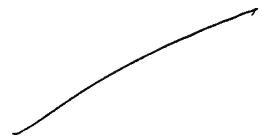
L8 ANSWER 12 OF 77 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 119:117172 CA
TITLE: Reaction of 2-acylcylohexane-1,3-diones with 6-hydrazinophenanthridine
AUTHOR(S): Rubinov, D. B.; Mikhailovsky, A. G.; Lahvich, F. A.
CORPORATE SOURCE: Inst. Tekh. Khim., Perm, 614600, Russia
SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (1992), (12), 1617-20
CODEN: KGSSAQ; ISSN: 0132-6244
DOCUMENT TYPE: Journal
LANGUAGE: Russian
GI



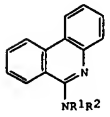
AB Condensation of cyclohexanediones I [R1 = Me, H, R2 = Me, Me(EtS)CHCH2, 1,3,5-Me3C6H2, R3 = H, CO2Me, R4 = Me, Pr, C11H23] with 6-hydrazinophenanthridine gave 79-91% enehydrazinoketones II; heating the reaction mixture caused cyclization to give 65-76% tetrahydroindazoles III [R1 = R2 = Me, R3 = H, R4 = Me, Pr; R1 = H, R2 = Me(EtS)CHCH2, R3 = H, R4 = Pr].
IT 144402-92-6, 6-Hydrazinophenanthridine
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with acylcyclohexanediones)
RN 144402-92-6 CA
CN 6(5H)-Phenanthridinone, hydrazone (9CI) (CA INDEX NAME)

L8 ANSWER 12 OF 77 CA COPYRIGHT 2005 ACS on STN (Continued)

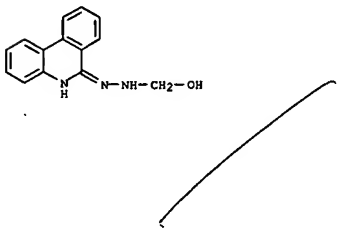




L8 ANSWER 13 OF 77 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 119:582 CA
TITLE: Synthesis, antiaggregation, and antiarrhythmic activity of phenanthridine derivatives
AUTHOR(S): Mikhailovsky, A. G.; Taranova, T. G.; Syropyatov, B. Ya.; Vakhrin, M. I.
CORPORATE SOURCE: Inst. Tekhn. Khim., Perm, Russia
SOURCE: Khimiko-Farmatsevticheskii Zhurnal (1992), 26(11-12), 53-5
CODEN: KHFZAN; ISSN: 0023-1134
DOCUMENT TYPE: Journal
LANGUAGE: Russian
GI

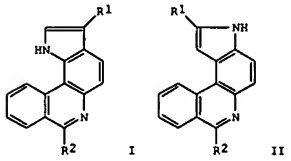


AB Phenanthridine derivs. (I, R1 = e.g., H, R2 = cyclohexyl, o-toluyl, NR1R2 = morpholino) were prepared by the reaction of 6-chlorophenanthridine with the corresponding amines. I showed blood platelet aggregation inhibitory and antiarrhythmic activities in mice.
IT 144402-93-7
RL: BIOL (Biological study)
(antiarrhythmic and blood platelet aggregation inhibitory activities of)
RN 144402-93-7 CA
CN 6(5H)-Phenanthridinone, (hydroxymethyl)hydrazone (9CI) (CA INDEX NAME)

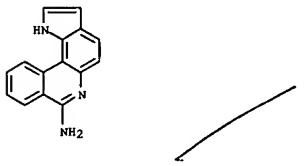


L8 ANSWER 14 OF 77 CA COPYRIGHT 2005 ACS on STN (Continued)

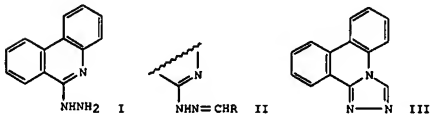
L8 ANSWER 14 OF 77 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 118:38800 CA
TITLE: Pyrrolophenanthridines. VI. Chemical properties of 1H-pyrrolo[2,3-a]phenanthridine and 3H-pyrrolo[3,2-a]phenanthridine
AUTHOR(S): Samoilova, M. E.; Buyanov, V. N.; Baberkina, E. P.; Bezrukov, I. A.; Suvorov, N. N.
CORPORATE SOURCE: Mosk. Khim.-Tekhnol. Inst., Moscow, Russia
SOURCE: Zhurnal Organicheskoi Khimii (1992), 28(4), 831-5
CODEN: ZORKAE; ISSN: 0514-7492
DOCUMENT TYPE: Journal
LANGUAGE: Russian
GI



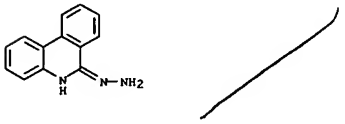
AB Pyrrolophenanthridines I and II (R1 = R2 = H) underwent electrophilic substitution (Vilsmeier, azo coupling, and Mannich reactions) and nucleophilic amination (Chichibabin reaction) to give the corresponding products I, II (R1 = CHO, p-O2NC6H4N:N, R2 = H; R1 = H, R2 = NH2) and I (R1 = Me2NCH2, R2 = NH2).
IT 145163-19-5, 1H-Pyrrolo[2,3-a]phenanthridin-7-amine
RL: RCT (Reactant); RACT (Reactant or reagent)
(substitution reactions of)
RN 145163-19-5 CA
CN 1H-Pyrrolo[2,3-a]phenanthridin-7-amine (9CI) (CA INDEX NAME)



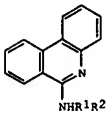
L8 ANSWER 15 OF 77 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 117:233824 CA
TITLE: Synthesis and properties of phenanthridine hydrazones
AUTHOR(S): Mikhailovskii, A. G.; Shklyaev, V. S.
CORPORATE SOURCE: Inst. Org. Khim., Perm, 614600, Russia
SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (1992), (4), 531-4
CODEN: KGSSAQ; ISSN: 0132-6244
DOCUMENT TYPE: Journal
LANGUAGE: Russian
GI



AB 6-Hydrazinophenanthridine (I), prepared in 93% yield from the corresponding chloro derivative, condensed with RCHO (R = Cl3C, substituted Ph, 2-furyl) and CH2O to give hydrazone II, but condensation with HCO2H gave triazolophenanthridine III.
IT 144402-92-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and condensation reactions with carbonyl compds.)
RN 144402-92-6 CA
CN 6(5H)-Phenanthridinone, hydrazone (9CI) (CA INDEX NAME)

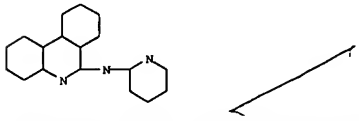


L8 ANSWER 16 OF 77 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 117:90108 CA
TITLE: Synthesis and alkylation of amidines of phenanthridine series
AUTHOR(S): Mikhailovskii, A. G.; Vakhrin, M. I.
CORPORATE SOURCE: Inst. Org. Khim., Perm, 614600, USSR
SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (1991), (10), 1361-4
CODEN: KGSSAQ; ISSN: 0453-8234
DOCUMENT TYPE: Journal
LANGUAGE: Russian
GI



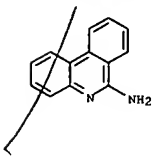
NHR1R2 I

AB Amination of 6-chlorophenanthridine by R1R2NH [R1 = H, R2 = PhCH2; R1R2 = (CH2)5, (CH2)2O(CH2)2] gave cyclic amidino derivs. I which were methylated by Me2SO4 to give the corresponding ammonium salts; similarly R3NH2 (R3 = aryl) gave I (R1 = H, R2 = aryl). Depending on the structure of the starting amidine alkylation may proceed at the exocyclic (N-alkyl), phenanthridine (N-aryl), or pyridine (N-2-pyridyl) N atom; in the case of I (R1 = H, R2 = 2-pyridyl).
IT 88783-61-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and quaternization by Me iodide)
RN 88783-61-3 CA
CN 6-Phenanthridinamine, N-2-pyridinyl- (9CI) (CA INDEX NAME)



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

L8 ANSWER 17 OF 77 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 116:173452 CA
TITLE: Resonance energies and tautomerism of substituted aromatic heterocycles and their benzo derivatives
AUTHOR(S): Yang, Pipeng; Duan, Wengui
CORPORATE SOURCE: Dep. Chem., Yunnan Univ., Kunming, 650091, Peop. Rep. China
SOURCE: Youji Huaxue (1991), 11(6), 620-3
CODEN: YCHHDX; ISSN: 0253-2786
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
AB The recently developed quantified resonance theory (QRT) has been applied to substituted aromatic five- and six-membered heterocycles and their benzo derivs. The calculated resonance energy differences ΔRE between tautomeric forms agree with those estimated from tautomeric equilibrium data for the 2- and 4-pyridone, 2-quinolone and 1-isoquinolone series. For tautomerism of extensive heteroarom. compds. in solution, the ΔRE and the differences in heats of atomization ΔΔH3 calculated by QRT can be used to rationalize and predict the predominant tautomer and the shifting trend in the equilibrium for a series of similar compds.
IT 832-68-8, 6-Phenanthridinamine
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)
(tautomerism of, resonance energy differences in)
RN 832-68-8 CA
CN 6-Phenanthridinamine (9CI) (CA INDEX NAME)



L8 ANSWER 18 OF 77 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 116:20919 CA
TITLE: Synthesis in the phenanthridine series. IV. Preparation of new radioprotectants with phenanthridine structure
AUTHOR(S): Lion, Claude; Boukou-Poba, Jean Paul; Charvy, Claude
CORPORATE SOURCE: Inst. Topol. Dyn. Syst., Univ. Paris 7, Paris, 75005, Fr.
SOURCE: Bulletin des Societes Chimiques Belges (1991), 100(2), 169-74
CODEN: BSCBAG; ISSN: 0037-9646
DOCUMENT TYPE: Journal
LANGUAGE: French
OTHER SOURCE(S): CASREACT 116:20919
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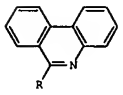
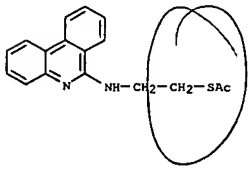
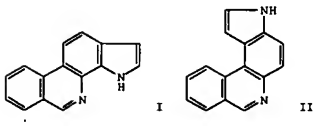


R I

AB New phenanthridines I (R = CH2CH2NHCH2CH2SAc, CH2CH2NMe2, CH:NCH2CH2SAc, NHCH2CH2SAc etc.) were easily obtained from I (R = Me) by a Mannich reaction, from I (R = Br) by substitution, or from I (R = CHO). These compds. are likely to be new radioprotectors.
IT 138118-78-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 138118-78-2 CA
CN Ethanethioic acid, S-[2-(6-phenanthridinylamino)ethyl] ester (9CI) (CA INDEX NAME)

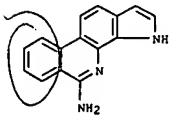


L8 ANSWER 19 OF 77 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 115:279858 CA
TITLE: Pyrrolophenanthridines. IV. Synthesis of 3H-pyrrolo[3,2-c]- and 3H-pyrrolo[3,2-a]phenanthridines. Reactivity of 3H-pyrrolo[3,2-c]phenanthridine
AUTHOR(S): Baberkina, E. P.; Samoilova, M. E.; Buyanov, V. N.; Akhvlediani, R. N.; Levina, I. I.; Bezrukov, I. A.; Suvorov, N. N.
CORPORATE SOURCE: Mosk. Khim.-Tekhnol. Inst., Moscow, USSR
SOURCE: Zhurnal Organicheskoi Khimii (1991), 27(5), 1110-18
CODEN: ZORKAE; ISSN: 0514-7492
DOCUMENT TYPE: Journal
LANGUAGE: Russian
GI



I II

AB The nitration of mixture of 1- and 3-methylphenanthridines gave 1-methyl-2-nitro- and 3-methyl-4-nitrophenanthridines, which in turn afforded pyrrolophenanthridines I and II, resp., on treatment with (EtO)2CHNMe2 in DMF in presence or absence of pyrrolidine, followed by cyclization with Zn/AcOH according to Lemgruber. II was also obtained in low yield in Fisher reaction from 2-aminophenanthridine. The aminomethylation, formylation and amination of I were studied.
IT 137531-26-1P, 3H-Pyrrolo[3,2-c]phenanthridin-5-amine
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 137531-26-1 CA
CN 3H-Pyrrolo[3,2-c]phenanthridin-5-amine (9CI) (CA INDEX NAME)



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L8          77 L7 AND PY<1998

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L8 ANSWER 20 OF 77 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 113:191251 CA
TITLE: A synthesis of 1,2,4-triazolo[1,5-f]phenanthridines by rearrangements of 1,2,5-oxadiazoles involving an NCN sequence with the imine nitrogen in an aromatic heterocyclic ring
AUTHOR(S): Cusmano, Giuseppe; Macaluso, Gabriella; Gruttadauria, Michelangelo; Buscemi, Silvestre
CORPORATE SOURCE: Dip. Chim. Org., Univ. Palermo, Palermo, 90123, Italy
SOURCE: Heterocycles (1990), 31(5), 869-75
CODEN: HTCYAM; ISSN: 0385-5414
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 113:191251
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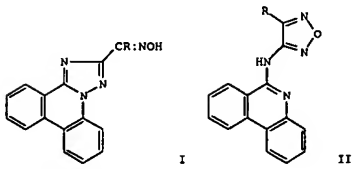
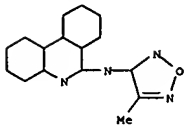


I II

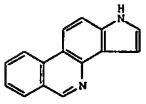
AB A synthetic pathway to the triazolophenanthridine system, e.g. (I; R = Me, Ph) by a base-catalyzed rearrangement of (phenanthridinylamino)oxadiazoles (II) has been investigated. This ring transformation is the first example of the applicability of the mononuclear heterocyclic rearrangement involving an NCN sequence to the synthesis of bridged nitrogen systems.
IT **130137-89-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and base-catalyzed rearrangement of)
RN 130137-89-2 CA
CN 6-Phenanthridinamine, N-(4-methyl-1,2,5-oxadiazol-3-yl)- (9CI) (CA INDEX NAME)

L8 ANSWER 20 OF 77 CA COPYRIGHT 2005 ACS on STN (Continued)



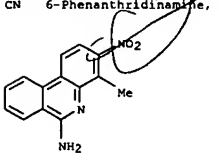
ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

L8 ANSWER 21 OF 77 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 113:78196 CA
TITLE: Pyrrolophenanthridines. III. New method of 1H-pyrrolo[2,3-c]phenanthridine synthesis
AUTHOR(S): Baberkina, E. P.; Akhvlediani, R. N.; Buyanov, V. N.; Samoilova, M. E.; Levina, I. I.; Suvorov, N. N.
CORPORATE SOURCE: Mosk. Khim.-Tekhnol. Inst., Moscow, USSR
SOURCE: Zhurnal Organicheskoi Khimii (1990), 26(2), 445-50
CODEN: ZORKAE; ISSN: 0514-7492
DOCUMENT TYPE: Journal
LANGUAGE: Russian
OTHER SOURCE(S): CASREACT 113:78196
GI

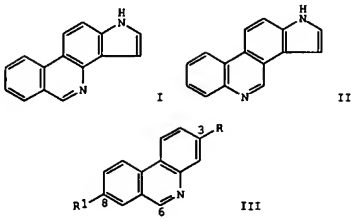


I

AB 4-Methyl-3-nitro- (I), 2-methyl-1-nitro-, and 2-methyl-3-nitrophenanthridines were prepared by cyclization of 2-[(2-chlorobenzylidene)amino]-6- and 4-[(2-chlorobenzylidene)amino]-2-nitrotoluene on reaction with Na-NH3(l). Treating I with Me2NCH(OEt)2 in DMF-containing Et3N followed by reduction of the intermediate enamine by Zn-AcOH gave pyrrolophenanthridine II.
IT **128422-33-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 128422-33-3 CA
CN 6-Phenanthridinamine, 4-methyl-3-nitro- (9CI) (CA INDEX NAME)



L8 ANSWER 22 OF 77 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 107:236551 CA
TITLE: Pyrrolophenanthridines. I. Synthesis and proton and carbon-13 NMR of 1H-pyrrolo[2,3-c]- and -[3,2-i]phenanthridines
AUTHOR(S): Frolov, E. P.; Akhvlediani, R. N.; Krasnokutskii, S. N.; Kurkovskaya, L. N.; Suvorov, N. N.
CORPORATE SOURCE: Mosk. Khim.-Tekhnol. Inst., Moscow, USSR
SOURCE: Zhurnal Organicheskoi Khimii (1987), 23(1), 189-95
CODEN: ZORKAE; ISSN: 0514-7492
DOCUMENT TYPE: Journal
LANGUAGE: Russian
OTHER SOURCE(S): CASREACT 107:236551
GI

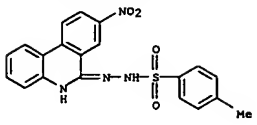


I II

III

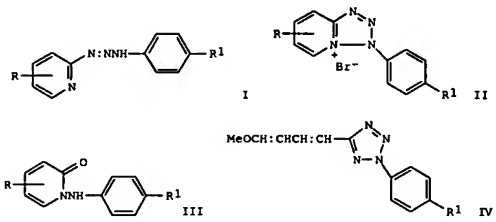
AB The novel heterocyclic compds. I and II were prepared from aminophenanthridines III (R = NH2, R1 = H; R = H, R1 = H2N) by successive diazotization-reduction with HONO-SnCl2 to give the corresponding hydrazine derivs., condensation with MeCOCO2H to give III (R, R1 = NHN:CMeCO2H, H) and cyclization with ZnCl2. The starting III were prepared in 3 steps from the corresponding 3-nitro-6-chloro- and 8-nitro-6-chloro derivs.
IT **111609-75-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and elimination reaction of)
RN 111609-75-7 CA
CN Benzenesulfonic acid, 4-methyl-, 2-(8-nitro-6-phenanthridinyl)hydrazide (9CI) (CA INDEX NAME)

L8 ANSWER 22 OF 77 CA COPYRIGHT 2005 ACS on STN (Continued)



L8 ANSWER 23 OF 77 CA COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 107:39697 CA
TITLE: Fused azolium salts. Part 8. Synthesis and nitrogen elimination of 3-aryltetrazolo(1,5-a)pyridinium salts and their angular benzenologs. Formation of N-arylamino-α-pyridones, -quinolones, -isoquinolones, and phenanthridones
AUTHOR(S): Messmer, A.; Gelleri, A.; Hajos, Gy.
CORPORATE SOURCE: Cent. Res. Inst. Chem., Hung. Acad. Sci., Budapest, H-1525, Hung.
SOURCE: Tetrahedron (1986), 42(17), 4827-36
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 107:39697
GI

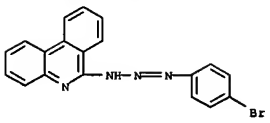


AB 2-Pyridylaryltriazenes I (R = H, 3-Me, 4-Me, 5-Me, 6-Me; R1 = H, OMe, Br, Cl) as well as 1-isoquinolyl-, 2-quinolyl and 6-phenanthridyltriazenes undergo cyclization in the presence of 2,4,6-tribromocyclohexa-2,5-dien-1-one to give 46-87% 3-aryltetrazolo[1,5-a]pyridinium salts II and their benzo analogs. These underwent N elimination with Et4N+OH- to give arylaminopyridinones III. Treatment of II with MeONa gave III together with the tetrazolylbutadiene esters IV.

IT 108999-40-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and ring closure of)

RN 108999-40-2 CA
CN Phenanthridine, 6-[3-(4-bromophenyl)-1-triazenyl]- (9CI) (CA INDEX NAME)

L8 ANSWER 23 OF 77 CA COPYRIGHT 2005 ACS on STN (Continued)



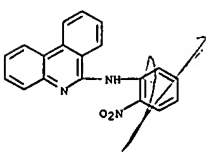
L8 ANSWER 24 OF 77 CA COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 104:19543 CA
TITLE: Intramolecular reaction between nitro and carbodiimide groups: a new synthesis of 2-arylbenzotriazoles
AUTHOR(S): Houghton, Peter G.; Pipe, David F.; Rees, Charles W.
CORPORATE SOURCE: Dep. Chem., Imp. Coll. Sci. Technol., London, SW7 2AY, UK
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1985), (7), 1471-9
CODEN: JCPRB4; ISSN: 0300-922X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 104:19543

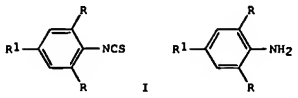
AB On heating in a number of solvents, tetrazole I decomposed to give N, CO2, and 80-90% 2-phenylbenzotriazole (II). This rearrangement proceeds via (2-nitrophenyl)phenylcarbodiimide (III). A number of other precursors of III, and III itself, all gave II on heating. This reaction is general for all o-NO2-substituted diarylcarbodiimides and their precursors. The reaction mechanism involves a sequence of electrocyclic ring closing and opening reactions.

IT 82937-37-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, reduction, and diazotization of)

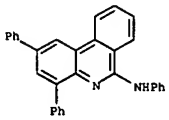
RN 82937-37-9 CA
CN 6-Phenanthridinamine, N-(2-nitrophenyl)- (9CI) (CA INDEX NAME)



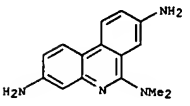
L8 ANSWER 25 OF 77 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 102:112954 CA
TITLE: Metathesis of aryl isothiocyanates: a novel method for the synthesis of sterically hindered aryl isothiocyanates
AUTHOR(S): Habib, Nargues S.; Rieker, Anton
CORPORATE SOURCE: Inst. Org. Chem., Univ. Tuebingen, Tuebingen, D-7400, Fed. Rep. Ger.
SOURCE: Synthesis (1984), (10), 825-7
CODEN: SYNTBF; ISSN: 0039-7881
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 102:112954
GI



AB Isothiocyanates I (R = alkyl, Ph, iodo; R1 = alkyl, H, OMe, Ph, iodo) were
prepared from anilines II and PhNCS. A mixture of II (R = R1 = Me) and PhNCS
was refluxed to give I (R = R1 = Me) and some PhNHCSNHPh.
IT 95096-34-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 95096-34-7 CA
CN 6-Phenanthridinamine, N,2,4-triphenyl- (9CI) (CA INDEX NAME)



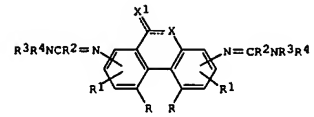
L8 ANSWER 26 OF 77 CA COPYRIGHT 2005 ACS on STN (Continued)
amino; R2 = H, (un)substituted alkyl; R3, R4 = alkyl, R3R4N = heterocyclyl; X = O, N, NH; X1 = O, H, halo, alkoxy, amino, heterocyclyl; dotted lines represent optional double bonds] were prepd. Thus, 3,8 diamino-5(6H)-phenanthridinone was stirred 30 min at room temp. with POCl3/AcNMe2 to give 85% phenanthridinediylbis[acetamidine] II. I are effective in vitro protozoacides against Entamoeba histolytica at 50-200 mcg/L.
IT 93494-47-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with amides)
RN 93494-47-4 CA
CN 3,6,8-Phenanthridinetriamine, N6,N6-dimethyl- (9CI) (CA INDEX NAME)



L8 ANSWER 26 OF 77 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 102:6224 CA
TITLE: Polycyclic bisamidines and their use as chemotherapeutic agents
INVENTOR(S): Bajwa, Balbir Singh; Chatterjee, Dipak Kumar; Ganguli,
Bimal Naresh; Reden, Juergen; DeSouza, Noel John
PATENT ASSIGNEE(S): Hoechst A.-G. , Fed. Rep. Ger.
SOURCE: Ger. Offen., 31 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3305329	A1	19840823	DE 1983-3305329	19830217
<--				
EP 117467	A1	19840905	EP 1984-101373	19840210
<--				
EP 117467	B1	19870506		
R: CH, DE, FR, GB, IT, LI				
US 4599409	A	19860708	US 1984-580181	19840215
<--				
AU 8424660	A1	19840823	AU 1984-24660	19840216
<--				
JP 59163371	A2	19840914	JP 1984-26195	19840216
<--				
ZA 8401138	A	19840926	ZA 1984-1138	19840216
<--				
PRIORITY APPLN. INFO.:			DE 1983-3305329 A	19830217

OTHER SOURCE(S): CASREACT 102:6224
GI



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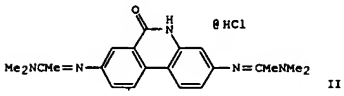
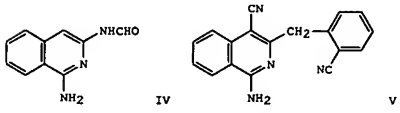


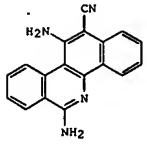
II

AB The title compds. [I; R = H, R2 = OC(O); R1 = H, alkyl, alkoxy, halo, NO2,

L8 ANSWER 27 OF 77 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 99:175557 CA
TITLE: Heterocyclic imines and amines. Part 18. Conversion of o-cyanobenzyl cyanide into isoquinoline, benzylisoquinoline, and azachrysene products
AUTHOR(S): Bardard, Ian F.; Elvidge, John A.
CORPORATE SOURCE: Chem. Dep., Univ. Surrey, Guildford, GU2 5XH, UK
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1983), (6), 1137-40
CODEN: JCPRB4; ISSN: 0300-922X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 99:175557
GI



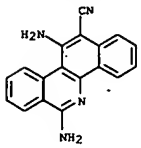
IV V



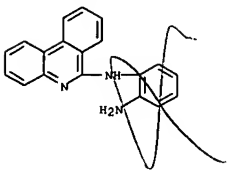
VI

AB Treatment of 2-NCC6H4CH2CN (I) with NaNH2 in ice-cold HCONH2 under N2 for 2 h gave the dimers 2-NCC6H4CH(CN)C(:NH)CH2C6H4CN-2 (II) and 2-NCC6H4CH(CN)C(:NH)C6H4CH2CN-2 (III), and the HCONH2 adduct IV. II underwent cycloisomerization to give the isoquinoline V whereas III gave the benzo[c]phenanthridine VI. Treatment of I with NaOMe in refluxing MeOH for 8 h gave 5% V; a similar reaction in refluxing DMSO/MeOH for 2 h under N2 gave 44% V.
IT 87606-65-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 87606-65-3 CA
CN Benzo[c]phenanthridine-12-carbonitrile, 6,11-diamino- (9CI) (CA INDEX NAME)

L8 ANSWER 27 OF 77 CA COPYRIGHT 2005 ACS on STN (Continued)

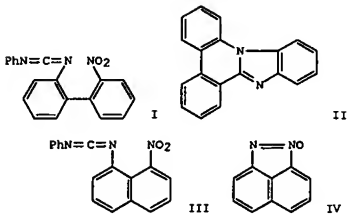


L8 ANSWER 28 OF 77 CA COPYRIGHT 2005 ACS on STN (Continued)



L8 ANSWER 28 OF 77 CA COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 97:127560 CA
TITLE: New rearrangements in the pyrolysis of nitrocarbodiimides
AUTHOR(S): Pipe, David F.; Rees, Charles W.
CORPORATE SOURCE: Dep. Chem., Imp. Coll. Sci. Technol., London, SW7 2AY, UK
SOURCE: Journal of the Chemical Society, Chemical Communications (1982), (9), 520-1
CODEN: JCCCAT; ISSN: 0022-4936
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 97:127560
GI



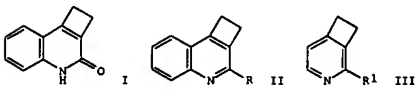
AB Flash vacuum pyrolysis of the nitrobiphenylcarbodiimide I gave 45% phenanthridine II, whereas similar treatment of the nitronaphthylcarbodiimide III gave 70% benzindazole N-oxide IV. Initially, intramol. nucleophilic attack by the O of the nitro group on the carbodiimide C occurs but the paths subsequently diverge to form 5-membered heterocyclic rings by different routes.

IT 82937-38-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and diazotization of)

RN 82937-38-0 CA
CN 1,2-Benzenediamine, N-6-phenanthridinyl- (9CI) (CA INDEX NAME)

L8 ANSWER 29 OF 77 CA COPYRIGHT 2005 ACS on STN

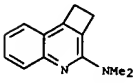
ACCESSION NUMBER: 97:55658 CA
TITLE: Cycloadditions in syntheses. VIII. Synthesis of 1,2-dihydrocyclobuta[c]pyridine and -quinoline and their 3-substituted derivatives
AUTHOR(S): Kaneko, Chikara; Naito, Toshihiko; Momose, Yu; Fujii, Harue; Nakayama, Nayomi; Koizumi, Ikue
CORPORATE SOURCE: Fac. Pharm. Sci., Kanazawa Univ., Kanazawa, 920, Japan
SOURCE: Chemical & Pharmaceutical Bulletin (1982), 30(2), 519-25
CODEN: CPBTAL; ISSN: 0009-2363
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 97:55658
GI



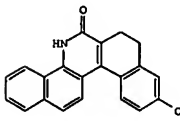
AB 1,2-Dihydrocyclobuta[c]quinolin-3(4H)-one (I) was prepared from 4-methoxyquinolin-2(1H)-one by photoaddn. of the latter to C2H4 and subsequent elimination of MeOH from the adduct. Chlorination of I with POCl3 gave 3-chloro derivative II (R = Cl), which then afforded either the parent base II (R = H) by reductive dechlorination, or 3-substituted derivs. II (R = MeO, MeS, Me2N, morpholino) by reaction with nucleophiles. The corresponding 1,2-dihydrocyclobuta[c]pyridine derivs. III (R1 = H, Cl, PhCH2O, MeO, EtS) were synthesized analogously.

IT 82450-10-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 82450-10-0 CA
CN Cyclobuta[c]quinolin-3-amine, 1,2-dihydro-N,N-dimethyl- (9CI) (CA INDEX NAME)



L8 ANSWER 30 OF 77 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 94:121256 CA
TITLE: Synthesis of some heterocycles via enamines from 6-methoxy-1-tetralone and benzo[f]chroman-4-one
AUTHOR(S): Sharma, S. D.; Manuja, Sushma; Gauba, A. L.
CORPORATE SOURCE: Dep. Chem., Panjab Univ., Chandigarh, 160 014, India
SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1980), 19B(4), 246-9
CODEN: IJSBDB; ISSN: 0376-4699
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 94:121256
GI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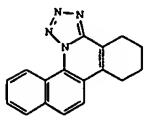
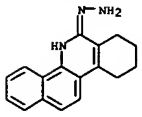

III

AB Reaction of 6-methoxy-1-tetralone and benzo[f]chroman-4-one with morpholine in the presence of TiCl4 gives the resp. enamines in high yields. Treatment of these enamines with aryl isocyanates/isothiocyanates affords the corresponding lactams, e.g. I. I on refluxing with POCl3 for 30 min gives fully aromatised 6-chloro-10-methoxydibenzo[c,k]phenanthridin e. Nucleophilic substitution of the halogen atom of 6-chloro-7,8,9,10-tetrahydrobenzo[c]phenanthridine with H2NNH2 yields the corresponding 6-hydrazino derivative, which on treatment with HNO2 undergoes cyclization to give the benzotetrazolophenanthridine III.

IT 76489-29-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclization of)

RN 76489-29-7 CA
CN Benzo[c]phenanthridin-6(5H)-one, 7,8,9,10-tetrahydro-, hydrazone (9CI) (CA INDEX NAME)

L8 ANSWER 30 OF 77 CA COPYRIGHT 2005 ACS on STN (Continued)



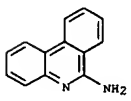
L8 ANSWER 31 OF 77 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 89:191671 CA
TITLE: Structural requirements for mutagenic activities of N-heterocyclic bases in the Salmonella test system
AUTHOR(S): Matsumoto, Takashi; Yoshida, Daisuke; Mizusaki, Shigenobu; Tomita, Hideo; Koshimizu, Koichi
CORPORATE SOURCE: Cent. Res. Inst., Japan Tob. and Salt Public Corp., Yokohama, Japan
SOURCE: Agricultural and Biological Chemistry (1978), 42(4), 861-4
CODEN: ABCHA6; ISSN: 0002-1369
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The mutagenic activities of quinoline [91-22-5], isoquinoline [119-65-3], phenanthridine [229-87-8], benzo[f]quinoline [85-02-9], benzo[h]quinoline [230-27-3], and their α-amino derivs. were compared in relation to the effects of structural changes using the S. typhimurium test system. All mutagenic compds. tested required the liver microsomal fraction for their mutagenic activity. Phenanthridine, two benzoquinolines, and quinoline were mutagenic. α-Amination of two benzoquinolines and quinoline increased their mutagenic activity intensively. Addition of a benzene ring to the benzene moiety of 2-aminoquinoline, so that two carbon atoms were shared, affected the increase in the mutagenic activity. Norharman [244-63-3] increased the mutagenicity of 2-aminobenzo[f]quinoline [36193-75-6].

IT 67419-74-3
RL: ADV (Adverse effect, including toxicity); BIOL (Biological study)
(mutagenicity of)

RN 67419-74-3 CA
CN 6-Phenanthridinamine, mixt. with benzo[h]quinoline (9CI) (CA INDEX NAME)

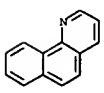
CM 1

CRN 832-68-8
CMF C13 H10 N2



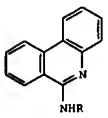
CM 2

CRN 230-27-3
CMF C13 H9 N



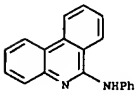
L8 ANSWER 31 OF 77 CA COPYRIGHT 2005 ACS on STN (Continued)

L8 ANSWER 32 OF 77 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 88:169929 CA
TITLE: The cyclodesulfurization of thio-compounds. Part 15. Synthesis of 6-substituted aminophenanthridines from some thiourea derivatives
AUTHOR(S): Omar, A. Mohsen M. E.; Habib, N. S.; Aboulwafa, Omaima M.
CORPORATE SOURCE: Fac. Pharm., Univ. Alexandria, Alexandria, Egypt
SOURCE: Pharmazie (1977), 32(12), 758-61
CODEN: PHARAT; ISSN: 0031-7144
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 88:169929
GI

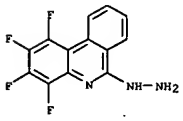


I

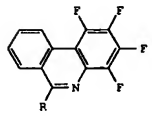
AB Phenanthridines I (R = 3-MeC6H4, 2-MeOC6H4, 4-ClC6H4, Ph, PhCH2, Bu) were prepared by treating 2-PhC6H4NH2 with RNCS and cyclizing 2-PhC6H4NHCSNHR with HgCl2, POCl3, or polyphosphoric acid. The best yields were obtained with POCl3. The HgCl2 complex of I·HCl (R = 3-MeC6H4) was also isolated.
IT 846-62-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 846-62-8 CA
CN 6-Phenanthridinamine, N-phenyl- (9CI) (CA INDEX NAME)



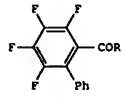
L8 ANSWER 33 OF 77 CA COPYRIGHT 2005 ACS on STN (Continued)



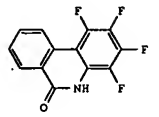
L8 ANSWER 33 OF 77 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 87:5778 CA
TITLE: Synthesis of derivatives of 1,2,3,4-tetrafluorophenanthridine
AUTHOR(S): Fomenko, T. V.; Gerasimova, T. N.; Fokin, E. P.
CORPORATE SOURCE: Novosib. Inst. Org. Khim., Novosibirsk, USSR
SOURCE: Izvestiya Sibirskogo Otdeleniya Akademii Nauk SSSR, Seriya Khimicheskikh Nauk (1977), (1), 99-102
CODEN: IZSKAB; ISSN: 0002-3426
DOCUMENT TYPE: Journal
LANGUAGE: Russian
GI



I



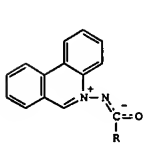
II



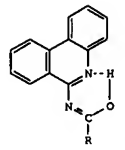
V

AB The phenanthridines I (R = Cl, piperidino, NHNH2, etc.) were prepared from
II (R = OH), which was treated with SOCl2, then with NaN3 to give II (R = N3) (III). Reaction of III with boiling EtOH, boiling C6H6/HCl, and CCl4 (20°) gave 2-PhC6F4NHCO2Et, (2-PhC6F4NH)2CO, and 2-PhC6F4NCO (IV), resp. Cyclization of IV with AlCl3/PhCl gave V, which reacted with POCl3 to give I (R = Cl) (VI). Treatment of VI with piperidine and hydrazine gave I (R = piperidino) and I (R = NHNH2), resp.
IT 62799-19-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 62799-19-3 CA
CN 6(5H)-Phenanthridinone, 1,2,3,4-tetrafluoro-, hydrazone (9CI) (CA INDEX NAME)

L8 ANSWER 34 OF 77 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 86:188776 CA
TITLE: Electron deficient heteroaromatic ammonioamidates. XII. The synthesis and photoisomerization of N-(5-phenanthridinio)benzamidates
AUTHOR(S): Agai, B.; Lempert, K.; Hegedus-Vajda, J.
CORPORATE SOURCE: Dep. Org. Chem., Tech. Univ. Budapest, Budapest, Hung.
SOURCE: Acta Chimica Academiae Scientiarum Hungaricae (1976), 91(1), 91-5
CODEN: ACASA2; ISSN: 0001-5407
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 86:188776
GI

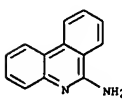


II



III

AB Amination of phenanthridine with 2,4,6-Me3C6H2SO3NH2 gave 5-aminophenanthridinium mesitylenesulfonate, aroylation of which gave the 5-(diaroylamino) analog (I). Partial dearoylation of I gave II (R = Ph, 4-ClC6H4, 4-MeOC6H4, or 4-O2NC6H4), which isomerized under UV irradiation to
give the N-6-phenanthridinylbenzimidic acids III. The stability of III was due to N...HO H-bonding.
IT 832-68-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 832-68-8 CA
CN 6-Phenanthridinamine (9CI) (CA INDEX NAME)

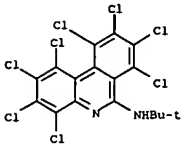


L8 ANSWER 35 OF 77 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 85:94204 CA
TITLE: Polyhaloheterocyclic compounds. Part XXIX. Perchloro-acridine, -phenanthridine, and -benzo[h]quinoline
AUTHOR(S): Chambers, Richard D.; Daniels, Richard; Musgrave, W. Kenneth R.; Russell, Peter L.
CORPORATE SOURCE: Dep. Chem., Univ. Durham, Durham, UK
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1976), (10), 1069-73
CODEN: JCPRB4; ISSN: 0300-922X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 85:94204

AB Perchloroacridine (I), -phenanthridine (II), and -benzo[h]quinoline were prepared by direct chlorination of the corresponding heterocycle or its monochloro derivative Attempts to replace Cl by F were unsuccessful. Hydrolysis of I and II gave the 9-acridone and phenthridin-6-one, resp. Nucleophilic substitution of I and II occurred at C-9 and C-6, resp.

IT 60159-57-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrolysis of)

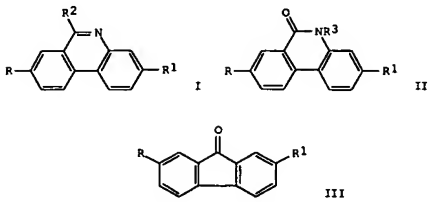
RN 60159-57-1 CA
CN 6-Phenanthridinamine, 1,2,3,4,7,8,9,10-octachloro-N-(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)



L8 ANSWER 36 OF 77 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 84:135502 CA
TITLE: Phenanthridines and phenanthridinones as antiviral agents
INVENTOR(S): Gauthier, George J.
PATENT ASSIGNEE(S): Pfizer Inc., USA
SOURCE: U.S., 13 pp. Division of U.S. 3,838,134.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3932643	A	19760113	US 1974-477529	19740607
<--				
US 3838131	A	19740924	US 1972-240830	19720403
<--				
US 3838134	A	19740924	US 1974-431255	19740107
<--				
PRIORITY APPLN. INFO.:			US 1972-240830	A3 19720403
			US 1974-431255	A3 19740107

GI

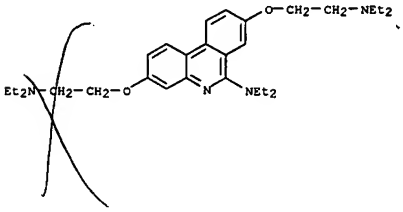


AB Phenanthridines I (R = R1 = Et2NCH2CH2O, (Me2CH)2NCH2CH2O; R2 = Cl, Et2N, PhCH2NH, MeO) and phenanthridinones II [R = H, R1 = Et2NCH2CH2O; R = Et2NCH2CH2O, R1 = H; R = R1 = Et2NCH2CH2O, Me2NCH2CH2CH2O, (Me2CH)2NCH2CH2O; R3 = H, Et2NCH2CH2] were prepared Ring expansion of fluorenone III by either a Schmidt reaction or a Beckmann rearrangement of its oxime gave II which was N-alkylated using R3X (X = halide) or was chlorinated using POCl3 and then condensed with R2H. Thus, III (R = R1 = Et2NCH2CH2O) was treated with HN3-H2SO4 to give II (R3 = H) (IV). IV when administered orally at 200 mg and 40 mg/kg to rats infected with

L8 ANSWER 36 OF 77 CA COPYRIGHT 2005 ACS on STN (Continued)
encephalomyocarditis virus gave had 72% and 28% survival resp., whereas the known antiviral agent, III (R = R1 = Et2NCH2CH2O) gave survival rates of 93% and 49%, survival resp.

IT 54153-44-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 54153-44-5 CA
CN 6-Phenanthridinamine, 3,8-bis[2-(diethylamino)ethoxy]-N,N-diethyl- (9CI) (CA INDEX NAME)



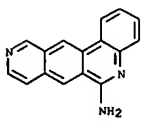
L8 ANSWER 37 OF 77 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 84:121588 CA
TITLE: Rearrangements in the photochemical synthesis of indolic compounds
AUTHOR(S): Riche, Claude; Chiaroni, Angele; Doucerain, Herve; Besselievre, Richard; Thal, Claude
CORPORATE SOURCE: Inst. Chim. Subst. Nat., Gif-sur-Yvette, Fr.
SOURCE: Tetrahedron Letters (1975), (51), 4567-70
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: French

GI For diagram(s), see printed CA Issue.

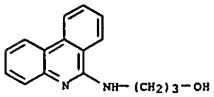
AB Irradiation of the indole I (R= CN, R1 = 1,2,5,6-N-methylpyridin-3-yl) in EtOH gave the spiroindole II and not a dihydroindole as previously stated (C. Dieng, et al, 1975). The structure of II was determined by x-ray anal. The B and C rings in II formed an envelope conformation, with ring D in the semi-chair conformation of cyclohexene. II was a precursor of aspidospermane-type alkaloids. Irradiation of the indole I (R = CN, R1 = 4-pyridyl) in EtOH gave 7-(o-anilino)isoquinoline-6-carbonitrile (III) and the fused compds. IV and V. Irradiation of I (R = CN, CO2Me, R1 = 4-pyridyl) under oxidative conditions gave dehydro analogs of IV. The structure of III was determined by x-ray anal.

IT 59171-78-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 59171-78-7 CA
CN Pyrido[4,3-j]phenanthridin-6-amine (9CI) (CA INDEX NAME)



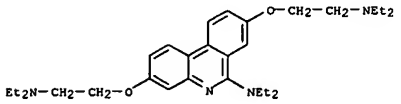
L8 ANSWER 38 OF 77 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 84:4856 CA
TITLE: Polycyclic fused amidines. I. Imidazo- and pyrimido[1,2-f]phenanthridines
AUTHOR(S): Cookson, Ronald F.; Rodway, Ronald E.
CORPORATE SOURCE: Nicholas Res. Lab., Slough, UK
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1975), (19), 1850-4
CODEN: JCPRB4; ISSN: 0300-922X
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB Phenanthridone (I; R = H) on heating with NH2(CH2)2N+H3 p-MeC6H4SO3- gave 2,3-dihydroimidazo[1,2-f]phenanthridine (II). The structure of II was confirmed by its synthesis from I [R = (CH2)2NH2] by thermolysis. Imidazo[1,2-f]phenanthridine was prepared by dehydrogenation of II or by the cycloaddn. of 6-chlorophenanthridine with NH2CH2CH(OMe)2. 6-(3-Hydroxypropylamino)phenanthridine, on heating with POCl3 gave 3,4-dihydro-2H-pyrimido[1,2-f]phenanthridine (III).
IT 38052-91-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclization of)
RN 38052-91-4 CA
CN 1-Propanol, 3-(6-phenanthridinylamino)- (9CI) (CA INDEX NAME)



L8 ANSWER 39 OF 77 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 81:169445 CA
TITLE: Phenanthridinones as antiviral agents
INVENTOR(S): Gauthier, George J.
SOURCE: U.S., 11 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3838134	A	19740924	US 1974-431255	19740107
<--				
US 3838131	A	19740924	US 1972-240830	19720403
<--				
US 3932643	A	19760113	US 1974-477529	19740607
<--				
PRIORITY APPLN. INFO.:			US 1972-240830	A3 19720403
			US 1974-431255	A3 19740107

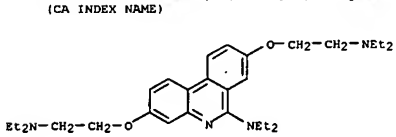
GI For diagram(s), see printed CA Issue.
AB Phenanthridinones I [R = R1 = OCH2CH2NEt2, O(CH2)3NMe2, OCH2CH2N(CHMe2)2; R = OCH2CH2NEt2, R1 = H; R = H, R1 = OCH2CH2NEt2; R2 = H, Me, CH2Ph, CH2CH2NEt2] were prepared by Schmidt reaction of the 9-fluorenones II with NaN3. Chlorination gave III (R3 = Cl, R4 = Et, CHMe2), which were aminated or alkoxylated to III (R3 = NEt2, NHCH2Ph, OMe). Thus, Schmidt reaction of 5 g II (R = R1 = CH2CH2NEt2) with 1.19 g NaN3 gave 1.57 g I (R = R1 = CH2CH2NEt2, R2 = H), which at 40 mg/kg orally caused 28% survival in encephalomyocarditis virus-infected mice.
IT 54153-44-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 54153-44-5 CA
CN 6-Phenanthridinamine, 3,8-bis[2-(diethylamino)ethoxy]-N,N-diethyl- (9CI) (CA INDEX NAME)



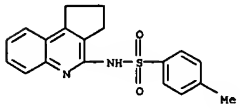
L8 ANSWER 40 OF 77 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 81:152029 CA
TITLE: Di(dialkylaminoalkoxy)phenanthridines as antiviral agents
INVENTOR(S): Gauthier, George J.
PATENT ASSIGNEE(S): Pfizer Inc.
SOURCE: U.S., 11 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3838131	A	19740924	US 1972-240830	19720403
<--				
US 3838134	A	19740924	US 1974-431255	19740107
<--				
US 3932643	A	19760113	US 1974-477529	19740607
<--				
PRIORITY APPLN. INFO.:			US 1972-240830	A3 19720403
			US 1974-431255	A3 19740107

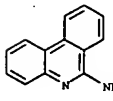
GI For diagram(s), see printed CA Issue.
AB Phenanthridinones I [R = R1 = OCH2CH2NEt2, O(CH2)3NMe2, OCH2CH2N(CHMe2)2; R = OCH2CH2NEt2, R1 = H; R = H, R1 = OCH2CH2NEt2; R2 = H, Me, CH2Ph, CH2CH2NEt2] were prepared by Schmidt reaction of the 9-fluorenones II with NaN3. Chlorination gave III (R3 = Cl, R4 = Et, CHMe2) which were aminated or alkoxylated to give III (R3 = NEt2, NHCH2Ph, OMe). Thus, Schmidt reaction of 5 g II (R = R1 = CH2CH2NEt2) with 1.19 g NaN3 gave 1.57 g I (R = R1 = CH2CH2NEt2, R2 = H), which at 40 mg/kg orally caused 28% survival in encephalomyocarditis virus-infected mice.
IT 54153-44-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 54153-44-5 CA
CN 6-Phenanthridinamine, 3,8-bis[2-(diethylamino)ethoxy]-N,N-diethyl- (9CI) (CA INDEX NAME)



L8 ANSWER 41 OF 77 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 79:146322 CA
TITLE: Reactions between arenesulfonyl azides and tetrahydrocarbazoles
AUTHOR(S): Bailey, A. Sydney; Buckley, Alan J.; Seager, John F.
CORPORATE SOURCE: Dyson Perrins Lab., Univ. Oxford, Oxford, UK
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1973), (17), 1809-18
CODEN: JCPRB4; ISSN: 0300-922X
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB The spiro compound (I) in F3CCO2H gave 1,2,3,4,4a,9a-hexahydro-9-methyl-4a-(p-tolylsulfonylamino)-9a-(trifluoroacetoxy)carbazolium trifluoroacetate which with Na2CO3 gave 2,3,4,4a-tetrahydro-9-methyl-4a-(p-tolylsulfonylamino)carbazole. The latter was an intermediate in the reaction of 4-MeC6H4SO2N3 and 9-methyltetrahydrocarbazole (II). Tetrahydrocarbazoles with arenesulfonyl azides in base gave cyclopentenoquinolines, e.g. II with 4-ClC6H4SO2N3 gave 80% imine (III). 1-Methyltetrahydrocarbazole with 4-Me- and 4-ClC6H4SO2N3 gave imine IV (R = Me and Cl, resp.). 1,9-Dimethyltetrahydrocarbazole with 4-MeC6H4SO2N3 gave sulfonamide V. The kinetics of the acid-catalyzed rearrangement of I were studied.
IT 50527-99-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 50527-99-6 CA
CN Benzenesulfonamide, N-(1,2,3,5-tetrahydro-4H-cyclopenta[c]quinolin-4-ylidene)-4-methyl- (9CI) (CA INDEX NAME)

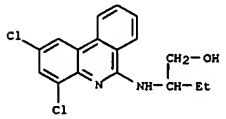


L8 ANSWER 42 OF 77 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 78:124536 CA
Correction of: 77:88439
TITLE: New synthesis of dihydroimidazo compounds
AUTHOR(S): Cookson, R. F.; Rodway, R. E.
CORPORATE SOURCE: Nicholas Res. Inst., Slough/Bucks., UK
SOURCE: Journal of the Chemical Society, Chemical Communications (1972), (9), 511-12
CODEN: JCCCAT; ISSN: 0022-4936
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB Phenanthridone or phthalazone was treated with H2N(CH2)2NH2.HS-O3C5H4Me-p at 200-250° to give the dihydroimidazo-fused systems (I and II resp.).
IT 40925-78-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 40925-78-8 CA
CN 1,2-Ethanediamine, N-6-phenanthridinyl-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

L8 ANSWER 43 OF 77 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 77:139956 CA
TITLE: Facile synthesis of 2,3-dihydroimidazo-and 1,2,3,4-tetrahydropyrimido[1,2-f]phenanthridines
AUTHOR(S): Pan, Hsi-Lung; Fletcher, T. Lloyd
CORPORATE SOURCE: Sch. Med., Univ. Washington, Seattle, WA, USA
SOURCE: Journal of Heterocyclic Chemistry (1972), 9(4), 859-64
CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB When 6-[2-(hydroxyethyl)amino-,6-(3-hydroxypropyl)amino-, or 6-[2-(1-hydroxybutyl) aminophenanthridines, dissolved in concentrated H2SO4, were treated with nitrosylsulfuric acid at 0-25°, then diluted with H2O and basified with aqueous NaOH at 65-86°, 2,3-dihydroimidazo-, 1,2,3,4-tetrahydropyrimido-, or 2,3-dehydro-2- ethylimidazo [1,2-f phenanthridines (I, II, and III, R1 = H, Cl, NO2, R2 = H, Cl, Br, R3 = H, Cl, Br, NO2, NH2, R4 = H, Cl, Br) were obtained resp. in good yields. Structures were substantiated by ir spectroscopy. The 6-ω-hydroxyalkylamino-phenanthridines were prepared from the 6-chlorophenanthridines. A possible mechanism for the formation of these ring systems is postulated.
IT 38040-74-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 38040-74-3 CA
CN 1-Butanol, 2-[(2,4-dichloro-6-phenanthridinyl)amino]- (9CI) (CA INDEX NAME)

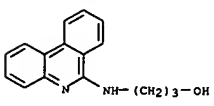


L8 ANSWER 44 OF 77 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 77:126598 CA
TITLE: Condensed nitrogen heterocycles
INVENTOR(S): Rodway, Ronald Ernest; Cookson, Ronald Frederick
PATENT ASSIGNEE(S): Aspro-Nicholas Ltd.
SOURCE: Ger. Offen., 57 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

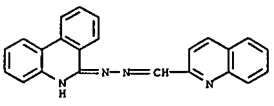
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2206012	A	19720824	DE 1972-2206012	19720209
GB 1347493	A	19740220	GB 1971-4457	19710211
CH 539643	A	19730914	CH 1972-1857	19720208
CH 539644	A	19730914	CH 1973-4310	19720208
BE 779128	A1	19720530	BE 1972-113762	19720209
FR 2125378	A5	19720929	FR 1972-4622	19720211
FR 2125378	B1	19750425		
US 3887566	A	19750603	US 1972-230464	19720229
SE 7413349	A	19741023	SE 1974-13349	19741023

PRIORITY APPLN. INFO.: GB 1971-4457 A 19710211

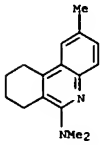
AB Compds. in the ring systems imidazo[1,2-a]quinoline, imidazo[2,1-a]phthalazine, imidazo[2,1-f]phenanthridine, imidazo[2,1-a]isoquinoline, imidazo[1,2-a]quinazoline, pyrimido[1,2-f]phenanthridine, indeno[1,2,3-de]pyrimido[2,1-a]phthalazine, imidazo[2,1-a]indeno[1,2,3-de]phthalazine, pyrimido[1,2-a]quinazoline, pyrimido[2,1-a]phthalazine, pyrimido[1,2-a]quinoline, pyrimido[1,2-a]quinoxaline, pyrimido[2,1-a]isoquinoline, imidazo[1,2-c]quinazoline (56) were prepared by ring-closure reaction of the ω-chloroalkylheterocycles.
IT 38052-91-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 38052-91-4 CA
CN 1-Propanol, 3-(6-phenanthridinylamino)- (9CI) (CA INDEX NAME)



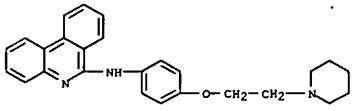
L8 ANSWER 45 OF 77 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 76:135311 CA
TITLE: Ligand structure and fluorescence of metal chelates. N-Heterocyclic hydrazones with zinc
AUTHOR(S): Ryan, D. E.; Snape, F.; Winpe, M.
CORPORATE SOURCE: Dep. Chem., Dalhousie Univ., Halifax, NS, Can.
SOURCE: Analytica Chimica Acta (1972), 58(1), 101-6
CODEN: ACACAM; ISSN: 0003-2670
DOCUMENT TYPE: Journal
LANGUAGE: English
AB -Benzimidazolecarboxaldehyde 2-quinolylhydrazone (I) is the most sensitive reagent of 15 N-containing heterocyclic hydrazones for the fluorimetric determination of Zn; <1 ppb Zn can be determined with excitation and emission wavelengths of 470 and 520 nm, resp. Efficiency ratios (ER), which are a measure of the effect of nonradiative processes which compete with fluorescence from the excited state, are given; pyridine-2-aldehyde 2-pyridylhydrazone, which shows slight fluorescence with Zn, has an ER of 0.4 + 10-4 whereas I, which fluoresces strongly on reacting with Zn has an ER of 1.538 + 10-7. Fluorescence intensity is greatest for those compds. which energetically prefer a -C:N- structural form.
IT 35896-20-9D, 2-Quinolinecarboxaldehyde, 6-phenanthridinylhydrazone, zinc complex
RL: PEP (Physical, engineering or chemical process); PROC (Process)
(fluorescence spectrum of)
RN 35896-20-9 CA
CN 2-Quinolinecarboxaldehyde, 6-phenanthridinylhydrazone (9CI) (CA INDEX NAME)



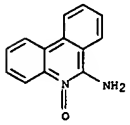
L8 ANSWER 46 OF 77 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 76:85668 CA
TITLE: Heterocyclic compounds. IV. Synthesis of some mono- and diazaphenanthrene derivatives
AUTHOR(S): Bose, Ajay K.; Manhas, M. S.; Rao, V. V.; Chen, C. T.; Trehan, I. R.; Sharma, S. D.; Amin, S. G.
CORPORATE SOURCE: Dep. Chem. Chem. Eng., Stevens Inst. Technol., Hoboken, NJ, USA
SOURCE: Journal of Heterocyclic Chemistry (1971), 8(6), 1091-4
CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 76:85668
GI For diagram(s), see printed CA Issue.
AB 6-Chlorotetrahydrophenanthridines (I, R = H, 2-OMe, 2-Me, 2-Cl, 2-Br; R1 = Cl, NMe2, NHMe, NHEt, H) were prepared as intermediates for the synthesis of antimalarials. A cyclohexanone enamine was treated with an aryl isocyanate to give quant. yields of enamides which gave ketoamides in acid. Cyclization yielded phenanthridones which reacted with POCl3 to give 6-substituted 7,8,9,10-tetrahydro-phenanthridines (I). Refluxing these products in an amide solution gave the N-substituted phenanthridines I (R = 4-Me, R1 = NMe2, NHMe, NHEt).
IT **35417-80-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 35417-80-2 CA
CN 6-Phenanthridinamine, 7,8,9,10-tetrahydro-N,N,2-trimethyl- (9CI) (CA INDEX NAME)



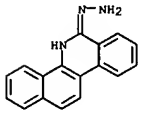
L8 ANSWER 47 OF 77 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 75:108210 CA
TITLE: Anticonvulsant activity of a series of phenanthridine basic ethers
AUTHOR(S): Ashford, A.; Brown, G. R.; Palmer, P. J.; Ross, J. W.; Trigg, R. B.; Ward, R. J.
CORPORATE SOURCE: Chem. Pharmacol. Sect., Twyford Lab. Ltd., London, UK
SOURCE: Arzneimittel-Forschung (1971), 21(7), 937-9
CODEN: ARZNAD; ISSN: 0004-4172
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB Twenty-two phenanthridine basic ethers (I), including 6-[m-(2-diethylaminoethoxy)phenyl]phenanthridine, 6-[p-(3-dimethylaminopropoxy)phenyl]phenanthridine, and 6-[p-(2-ethylaminoethoxy)phenyl]phenanthridine, showed potent anticonvulsant activity in mice against leptazol (II) and maximal electroshock convulsions, but neurotoxic activity was relatively high, precluding clin. use.
IT **34244-46-7**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(antispasmodic activity of)
RN 34244-46-7 CA
CN Phenanthridine, 6-(β-piperidino-p-phenetidino)- (8CI) (CA INDEX NAME)



L8 ANSWER 48 OF 77 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 66:104548 CA
TITLE: Intramolecular trapping of hydroxylamines from the catalytic hydrogenation of 2-nitrobiphenyls
AUTHOR(S): Muth, Chester W.; Elkins, J. R.; DeMatte, Michael L.; Chiang, S. T.
CORPORATE SOURCE: West Virginia Univ., Morgantown, WV, USA
SOURCE: Journal of Organic Chemistry (1967), 32(4), 1106-10
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 66:104548
GI For diagram(s), see printed CA Issue.
AB Catalytic hydrogenation of 2-nitro-2'-carboxybiphenyl (I) and its carboxy derivs. in ethanol in the presence of Pt has led to products resulting from the intramol. trapping of hydroxylamino and amino groups. In the presence of mineral acid the order of hydroxylamino trapping abilities is carbamoyl > carbomethoxy > carboxy. With no added mineral acid the order of trapping abilities is reversed. Compds. containing the cyano group were found to yield only hydroxylamino-trapped products.
IT **7605-77-8DP**, Phenanthridine, 6-amino-, 5-oxide, copper complex
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 7605-77-8 CA
CN Phenanthridine, 6-amino-, 5-oxide (6CI, 8CI) (CA INDEX NAME)



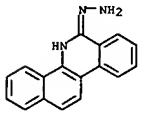
L8 ANSWER 49 OF 77 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 64:104193 CA
ORIGINAL REFERENCE NO.: 64:19603e-f
TITLE: Dibenzo[c,h]cinnoline oxides
AUTHOR(S): Poesche, W. H.
CORPORATE SOURCE: Univ. Alberta, Edmonton, Can.
SOURCE: Journal of the Chemical Society [Section] C: Organic (1966), (9), 890-3
CODEN: JSOOAX; ISSN: 0022-4952
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Dibenzo[c,h]cinnoline 5-oxide was synthesized. The compound is not identical with the H2O2 oxidation product of dibenzo[c,h]cinnoline and the Na2S reduction product of 1-nitro-2-o-nitrophenyl-naphthalene, which must therefore be dibenzo[c,h]cinnoline 6-oxide, as previously supposed. Aside from steric interactions, electronic effects are made responsible for the exclusive formation of the 6-oxide in the latter two cases.
IT **6091-67-4**, Benzo[c]phenanthridine, 6-hydrazino-
(preparation of)
RN 6091-67-4 CA
CN Benzo[c]phenanthridine, 6-hydrazino- (7CI, 8CI) (CA INDEX NAME)



L8 ANSWER 50 OF 77 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 64:104192 CA
ORIGINAL REFERENCE NO.: 64:19603b-e
TITLE: Valence tautomerism of heterocycles. VII. 3,4-Diazabicyclo[4.2.0]octa-2,4-diene derivative
AUTHOR(S): Maier, Guenther; Seidler, Friedrich
CORPORATE SOURCE: Tech. Hochsch., Karlsruhe, Germany
SOURCE: Chemische Berichte (1966), 99(4), 1236-40
CODEN: CHBEAM; ISSN: 0009-2940
DOCUMENT TYPE: Journal
LANGUAGE: German

AB cf. preceding abstrs. The preparation and properties of 1,6,7,8-tetramethyl-2,5-diphenyl-3,4-diazabicyclo[4.2.0]octa-2,4-diene (I) are described. 1,2,3,4-Tetramethyl-3-cyclobutene-1,2-dicarboxylic anhydride (2.00 g.) in AcOEt hydrogenated about 4 hrs. under ambient conditions over Pd-C yielded 1.82 g. anhydride (II) of 1,2,3,4-tetramethyl-cyclobutane-cis-1,2-dicarboxylic acid (III), m. 73-4° (petr. ether). II (2.00 g.) dissolved at about 60° in a slight excess dilute aqueous NaOH, filtered, and acidified with concentrated HCl precipitated 1.95 g. III, m. 150° (Et2O-petroleum ether). III (2.00 g.) in 70 cc. dry Et2O stirred 16 hrs. at room temperature with 5 mole equivs. PhLi-Et2O and poured into iced H2O, and the aqueous phase acidified with cold concentrated HCl gave 1.88 g. IV, m. 140-1° (CHCl3-petroleum ether). IV (1.00 g.) in 20 cc. Et2O with excess CH2N2-Et2O yielded 880 mg. Me 1,2,3,4-tetramethyl-cis-2-benzoylcyclobutane-1-carboxylate (V), b0.5 140°. V (1.00 g.) and 3 cc. N2H4.H2O in 150 cc. EtOH refluxed 4 days while treated after 24 and 48 hrs. with addnl. 2-cc. portions N2H4.H2O gave 810 mg. VI, m. 207° (EtOH). VI (1.00 g.) in 120 cc. dry tetrahydrofuran refluxed 3 hrs. with 3 mole equivs. PhLi-Et2O gave 760 mg. VII, m. 168° (AcOEt). VII (750 mg.) in 50 cc. Ac2O kept 12 hrs. and poured with cooling into dilute aqueous NaOH yielded 610 mg. yellow I, m. 174-5° (CH2Cl2-petroleum ether).

IT 6091-67-4, Benzo[c]phenanthridine, 6-hydrazino- (preparation of)
RN 6091-67-4 CA
CN Benzo[c]phenanthridine, 6-hydrazino- (7CI, 8CI) (CA INDEX NAME)

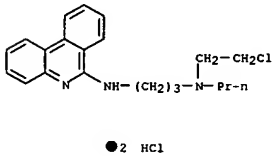


L8 ANSWER 51 OF 77 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 64:59793 CA
ORIGINAL REFERENCE NO.: 64:11173f-h,11174a
TITLE: Heterocyclic derivatives of 2-chloroethyl sulfide with antitumor activity
AUTHOR(S): Peck, Richard M.; O'Connell, Anna P.; Creech, Hugh J.
CORPORATE SOURCE: Inst. for Cancer Res., Philadelphia, PA
SOURCE: Journal of Medicinal Chemistry (1966), 9(2), 217-21
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English

GI For diagram(s), see printed CA Issue.

AB Several monofunctional nitrogen and sulfur mustards (e.g. I-V) combined with a variety of heterocyclic nuclei through aminoalkyl side chains were synthesized for comparisons of their antitumor activities. The presence of acridine, benz[c]acridine, and phenanthridine nuclei increased the antitumor effectiveness of both types of mustard moiety; the sulfur mustard derivs. displayed higher, but much broader, dosage ranges of activity. Since the sulfur mustards of 7-chloro- and 3,7-dichloroquinoline were considerably more effective against Ehrlich ascites tumors in the mouse than the corresponding nitrogen half-mustards, it is considered that studies utilizing sulfur mustard derivs. may be an improved procedure for the detection of potential antitumor activity in the carrier portion of the mol.

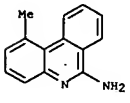
IT 4248-46-8, Phenanthridine, 6-[[3-[(2-chloroethyl)propylamino]propyl]amino]-, dihydrochloride (preparation of)
RN 4248-46-8 CA
CN 1,3-Propanediamine, N-(2-chloroethyl)-N'-6-phenanthridinyl-N-propyl-, dihydrochloride (9CI) (CA INDEX NAME)



L8 ANSWER 52 OF 77 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 63:24038 CA
ORIGINAL REFERENCE NO.: 63:4256e-f
TITLE: The phenanthridine series: preparation of some methylphenanthridines and amino derivatives
AUTHOR(S): Keene, B. R. T.; Tissington, P.
CORPORATE SOURCE: Medway Coll. Technol., Chatham, UK
SOURCE: Journal of the Chemical Society, Abstracts (1965), (May), 3032-7
CODEN: JCSAAZ; ISSN: 0590-9791
DOCUMENT TYPE: Journal
LANGUAGE: English

AB 1- and 10-Methyl and 1,10-dimethylphenanthridine have been synthesized. Amination of these bases, and 1,2- and 9,10-benzophenanthridine, gave the corresponding 6-amino derivatives. A partial resolution of 6-amino-1,10-dimethylphenanthridine has been achieved.

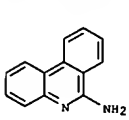
IT 1859-17-2, Phenanthridine, 6-amino-1-methyl- (preparation of)
RN 1859-17-2 CA
CN Phenanthridine, 6-amino-1-methyl- (7CI, 8CI) (CA INDEX NAME)



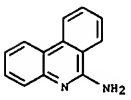
L8 ANSWER 53 OF 77 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 62:10081 CA
ORIGINAL REFERENCE NO.: 62:1883g-h
TITLE: Symposium on molecular action of mutagenic and carcinogenic agents. Acridine mutagens and DNA structure
AUTHOR(S): Lerman, L. S.
CORPORATE SOURCE: Med. Center, Univ. of Colorado, Denver
SOURCE: Journal of Cellular and Comparative Physiology (1964), 64(2;Pt. II;Suppl. 1), 1-13, discussion 13-18
CODEN: JCCPAY; ISSN: 0095-9898
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Evidence for intercalation of acridine compds. between 2 otherwise sequential base pairs was obtained by studies of sedimentation, low angle x-ray scattering, flow dichroism, flowpolarized fluorescence, and chemical reactivity. Such binding requires a local untwisting and extension of the double helix. The intercalated mols. have a decreased chemical reactivity. They increase the stability of the double helix as shown by an increase in the thermal transition temperature Intercalation into complexes formed between polyadenylic and polyuridylic acids makes the double helix more stable than the triple. Intercalation seems to be a prerequisite for mutagenicity of the insertion-deletion type but the acridine structure is not essential and not all intercalating mols. are mutagenic.

IT 832-68-8, Phenanthridine, 6-amino- (deoxyribonucleic acid structure and)
RN 832-68-8 CA
CN 6-Phenanthridinamine (9CI) (CA INDEX NAME)

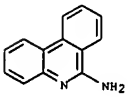


L8 ANSWER 54 OF 77 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 62:3105 CA
ORIGINAL REFERENCE NO.: 62:561d-e
TITLE: Cyclic Amidines. XVII. 4-Imino-1,2,3-benzotriazines
AUTHOR(S): Partridge, M. W.; Stevens, M. F. G.
CORPORATE SOURCE: Univ. Nottingham, UK
SOURCE: Journal of the Chemical Society, Abstracts (1964), (Oct.), 3663-9
CODEN: JCSAAZ; ISSN: 0590-9791
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB cf. CA 59, 5170e. 4-Imino-1,2,3-benzotriazines (I) afford, on reduction, 3-aminoindazoles (e.g. II) and on decomposition in acid, 6-aminophenan-thridines. The reactions of o-cyanophenyltriazenes were studied.
IT 832-68-8, Phenanthridine, 6-amino-
(preparation of)
RN 832-68-8 CA
CN 6-Phenanthridinamine (9CI) (CA INDEX NAME)

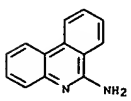


L8 ANSWER 55 OF 77 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 58:33285 CA
ORIGINAL REFERENCE NO.: 58:5635g-h,5636a-d
TITLE: Metal hydrazides. III. Amination of acridine and phenanthridine with sodium hydrazide and with sodium N,N-dimethylhydrazide
AUTHOR(S): Kauffmann, Thomas; Hacker, Herbert; Mueller, Horst
CORPORATE SOURCE: Tech. Hochschule, Darmstadt, Germany
SOURCE: Ber. (1962), 95, 2485-92
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 58:33285
GI For diagram(s), see printed CA Issue.
AB cf. CA 58, 2430f. The adducts from NaNHNH2 (I) or NaNHNMe2 (II) with acridine (III) or phenanthridine (IV) decomposed at 50-60° with elimination of NH3 or Me2NH, resp., and the formation of the Na salt of 9-aminoacridine (V) or 9-aminophenanthridine (VI), resp., in contrast to the corresponding adducts from C5H5N or isoquinoline (VII) which eliminate
H under the same conditions. The adduct from III and II yields upon hydrolysis the surprisingly stable 9-(N,N-dimethylhydrazino)-9,10-dihydroacridine (VIII). All reactions with I and II were performed under pure N. Anhydrous Me2NNH2 (5.05 g.) treated with 3.65 g. NaNH2 in 70 cc. 90%
C6H6 by the method previously described (CA 57, 7140h), the resulting suspension of 0.084 mole II treated dropwise with stirring at 0° with 5.0 g. III in 80 cc. C6H6, heated 4 hrs. at 60°, treated with 60 cc. H2O with cooling, and filtered yielded 5.4 g. (crude) V. III (5 g.) added with cooling to 0.084 mole II in the usual manner, stirred 2 hrs. with cooling, treated with cooling with 60 cc. H2O, and filtered, the
filtrate extracted with Et2O, and the filter residue and Et2O extract worked up
together gave 4.9 g. IX, m. 136-8° (Et2O at -60°), which kept 48 hrs. in a desiccator in vacuo decomposed to about 40% to III. II (0.084 mole) in 40 cc. C6H-treated dropwise during a few min. with 5.0 g. IV in 100 cc. C6H6, heated 4 hrs. at 60°, hydrolyzed with 100 cc. H2O with cooling, and worked up yielded 4.6 g. VI, m. 195° (EtOH). II (0.03 mole) and 0.03 mole Me2NNH2 in 60 cc. C6H6 treated with 2.6 g. VII, heated 4 hrs. at 70°, hydrolyzed with cooling with 20 cc. H2O, and saturated with K2CO3, and the organic phase worked up yielded 2.5 g. 1-(N,N-dimethylhydrazino)isoquinoline, m. 86° (Et2O); monopicrate m. 218-19° (EtOH). II (0.04 mole) in 80 cc. dry C6H6 treated at room temperature with a saturated solution of 2.0 g. 5,6-benzoquinoline in C6H6, heated
4 hrs. at 80°, and worked up gave 2.6 g. 2-(N,N-dimethylhydrazino)-5,6-benzoquinoline (X), m. 110° (petr. ether, b. 50-70°). 7,8-Benzoquinoline (3.6 g.) in C6H6 added at 5° to 0.06 mole II in 80 cc. dry C6H6, heated 3 hrs. at 80°, and worked up gave 3.6 g. yellow, viscous 7,8-isomer of X, b0.02 172-5°. III (5.0 g.) and 0.93 g. 99.2% N2H4 in 80 cc. C6H6 treated dropwise at 0° with 1.21 g. 90% NaNH2 in 70 cc. Et2O while being treated with a stream of N, heated
4 hrs. at 50°, treated with cooling with 50 cc. H2O, and filtered yielded 3.9 g. lemon-yellow crystals, m. 228-31°, which triturated 5 times with 50-cc. portions hot 2N HCl gave 89 mg. 9,10-dihydroacridine

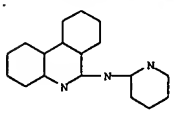
L8 ANSWER 55 OF 77 CA COPYRIGHT 2005 ACS on STN (Continued)
(XI), m. 170°; the filtrate satd. with K2CO3 and extd. with Et2O, and the residue (1.7 g.) from the ext. triturated twice with 50-cc. portions hot 2N HCl left 70 mg. XI; the HCl ext. from the filter residue satd. with K2CO3 pptd. 3.5 g. V, m. 232-3°; the ext. from the 2nd fraction satd. with K2CO3, and extd. with Et2O yielded 0.6 g. III. I (0.03 mole) treated in the usual manner with 0.03 mole IV in 60 cc. dry C6H6, heated 2 hrs. at 60°, and hydrolyzed with cooling with 20 cc. H2O gave 2% VI and 95% unchanged IV.
IT 832-68-8, Phenanthridine, 6-amino-
(preparation of)
RN 832-68-8 CA
CN 6-Phenanthridinamine (9CI) (CA INDEX NAME)



L8 ANSWER 56 OF 77 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 58:33284 CA
ORIGINAL REFERENCE NO.: 58:5635e-g
TITLE: Isothiocyanates. VIII. Study of the synthesis of diisothiocyanates and aminoisothiocyanates of acridine
AUTHOR(S): Kristian, P.; Antos, K.; Hulka, A.; Nemec, P.; Drobnica, L.
CORPORATE SOURCE: Sloven. Vysoka Skola Tech., Bratislava, Czech.
SOURCE: Chemicke Zvesti (1961), 15, 730-6
CODEN: CHZVAN; ISSN: 0366-6352
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB cf. CA 56, 12854e. The problem of the synthesis of 1-isothiocyanato-5-aminoacridine, 2-isothiocyanato-5-aminoacridine, 3-isothiocyanato-5-aminoacridine and 2,8-diisothiocyanatoacridine from the corresponding diaminoacridines is described. Because of the unreactivity of the 5-NH2 group in 5-aminoacridine it was expected that the other NH2 group would be
converted to isothiocyanate. For 1,5-(I), 2,5-(II) and 3,5-(III) diaminoacridine it was impossible to prepare the corresponding isothiocyanates. In I H bonds are formed between H on the hetero N with N
of of the 1-NH2 group. In II there is a possibility of the formation of a
p-quinoid structure from 2-NH2 group with the ionized form of the acridonimine. In III there is a possibility of the formation of an amino-imine tautomeric structure of the 3-NH2 group. The synthesis of a new compound, 2,8-diisothiocyanatoacridine, m. 200°, by the thiophosgene method is described.
IT 832-68-8, Phenanthridine, 6-amino-
(preparation of)
RN 832-68-8 CA
CN 6-Phenanthridinamine (9CI) (CA INDEX NAME)



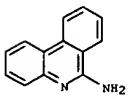
L8 ANSWER 57 OF 77 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 58:3220 CA
ORIGINAL REFERENCE NO.: 58:501h,502a-b
TITLE: The constitution of the red and colorless form of the quinolylmethanes. IV. Tautomerism and optical behavior of the quinolylamines
AUTHOR(S): Credner, Hans H.; Friedrich, Hans J.; Scheibe, Guenter
CORPORATE SOURCE: Tech. Hochschule, Munich, Germany
SOURCE: Ber. (1962), 95, 1881-93
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB cf. CA 57, 11162f. The quinolylamines, as did the corresponding methanes, existed in tautomeric forms and formed with suitable metal salts chelates which dissociated in basic solvents. The particular behavior of the proton was reflected in the absorption spectra. Di(2-pyridyl)amine (I) (4 g.) and excess MeI heated 2 hrs. at 90° in a sealed tube gave N,N'-dimethylpyridoazacyanine iodide (II), pale yellow needles, m. 290° (EtOH). I in absolute MeOH treated dropwise with stirring with 1 mole equivalent ZnCl2 in MeOH gave I.ZnCl2, m. above 360°. 9-Aminophenanthridine (III) (100 mg.) and 110 mg. 9-chlorophenanthridine (IV) fused together, boiled with alc. KOH, and filtered yielded 70% di(9-phenanthridyl)amine (V), yellow, m. 372° (HCONMe2). IV (0.5 g.) and 0.34 g. 2-aminoquinoline (VI) heated together and worked up in the same manner gave 20% 2-quinolyl-9-phenanthridylamine (VII), yellow, m. 204° (EtOH). IV (0.5 g.) and 0.22 g. 2-aminopyridine (VIII) gave similarly yellow 2-pyridyl-9-phenanthridylamine (IX). The ultraviolet absorption spectra of VIII, I, I.ZnCl2, VI, di(2-quinolyl)amine, N,N'-diethylquinoazacyanine iodide, III, IX, IX.ZnCl2, VII, VII.ZnCl2, V, V.ZnCl2, and II were recorded and evaluated.
IT 88783-61-3, Phenanthridine, 6-(2-pyridylamino)- (preparation of)
RN 88783-61-3 CA
CN 6-Phenanthridinamine, N-2-pyridinyl- (9CI) (CA INDEX NAME)



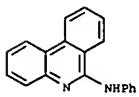
ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

L8 ANSWER 58 OF 77 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 55:144193 CA
ORIGINAL REFERENCE NO.: 55:27316c-h
TITLE: 6-Cyanophenanthridine and related compounds
AUTHOR(S): Hayashi, Eisaku; Ohki, Hideya
CORPORATE SOURCE: Shizuoka Coll. Pharm.
SOURCE: Yakugaku Zasshi (1961), 81, 1033-6
CODEN: YKKZAJ; ISSN: 0031-6903
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB 6-Cyanophenanthridine (I) (2 g.) in 30 ml. AcOH and 4 ml. 10.8% H2O2 heated 5 hrs. at 95-100°, cooled, and the product filtered off gave 2.1 g. I 5-oxide (II), needles, m. 216-17° (CHCl3-MeOH). Catalytic reduction of 0.3 g. II in 10 ml. each of C5H5N and MeOH with Raney Ni gave 0.17 g. I, m. 136-7°. I (1 g.) in 20 ml. C5H5N and 15 ml. 10.8% H2O2 treated with 1 g. K2CO3 in 10 ml. H2O and the product filtered off gave 0.9 g. 6-phenanthridinecarboxamide (III), needles, m. 190-2° (CHCl3). II (1 g.) in 20 ml. C5H5N treated with 10 ml. 10.8% H2O2, 0.7 g. K2CO3, and 7 ml. H2O, the mixture kept 1 hr. and the product filtered off gave 0.85 g. III 5-oxide (IV), needles, m. 283° (decomposition). III (0.5 g.) in 6 ml. AcOH and 1 ml. 10.8% H2O2 heated 5 hrs. at 95-100° and the product filtered off and washed with MeOH gave 0.25 g. IV, m. 283° (decomposition). I (0.4 g.) in 2.5 ml. concentrated H2SO4 and 0.2 ml. H2O heated 1 hr. at 95-100°, H2O added, and the mixture neutralized with NH4OH gave 0.35 g. III, needles, m. 190-2°. Similarly, hydrolysis of 0.4 g. II yielded 0.4 g. IV, m. 283° (decomposition). I (1 g.) in 6 ml. concentrated H2SO4 and 0.5 ml. H2O heated 1 hr. at 95-100°, the mixture cooled, treated dropwise with 0.5 g. NaNO2 in 3 ml. H2O, heated 30 min. at 95-100°, H2O added, and the product filtered off gave 1.1 g. phenanthridine-6-carboxylic acid (V), needles, m. 158° (MeOH). II (0.6 g.) in 3.5 ml. concentrated H2SO4 and 0.3 ml. H2O heated 1 hr. at 100° and the product filtered off gave 0.6 g. IV, m. 283° (decomposition). A solution of 0.4 g. KOH, 2 ml. H2O, 0.3 g. Br, and 0.4 g. IV heated 20 min. at 80°, the precipitate taken up in 10% HCl, filtered with C, and neutralized with NH4OH gave 0.25 g. 6-aminophenanthridine (VI), needles, m. 192-3°. Similarly, 0.6 g. IV yielded 0.15 g. VI 5-oxide, columns, m. 244-5°. V (0.4 g.) in 4 ml. AcOH and 0.8 ml. 10.8% H2O2 heated 5 hrs. at 100° gave 0.15 g. 6-hydroxyphenanthridine 5-oxide, m. 251-4° (C5H5N) and the mother liquor gave 0.1 g. phenanthridone, m. 288-90°. A mixture of 1.5 g. 6-phenoxyphenanthridine, 1.5 g. urea, and 5 g. PhOH heated 2 hrs. at 180°, cooled, 30 ml. 10% NaOH added, and the product filtered off gave 0.8 g. VI, m. 191-3°
IT 832-68-8, Phenanthridine, 6-amino- (preparation of)
RN 832-68-8 CA
CN 6-Phenanthridinamine (9CI) (CA INDEX NAME)

L8 ANSWER 58 OF 77 CA COPYRIGHT 2005 ACS on STN (Continued)

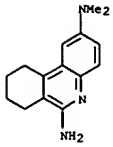


L8 ANSWER 59 OF 77 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 55:144186 CA
ORIGINAL REFERENCE NO.: 55:27311i,27312a-b
TITLE: Reaction of phenanthridine 5-oxide with phenyl isocyanate
AUTHOR(S): Hayashi, Eisaku
CORPORATE SOURCE: Shizuoka Coll. Pharm.
SOURCE: Yakugaku Zasshi (1961), 81, 1030-2
CODEN: YKKZAJ; ISSN: 0031-6903
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB Phenanthridine 5-oxide (I) (0.2 g.) in 10 ml. CHCl3 heated with 0.12 g. PhNCO and the product extracted with (Me2CH)2O gave 0.15 g. 6-anilinophenanthridine (II), plates, m. 152-4° (MeOH). 6(5H)-Phenanthridinone (5 g.) and 10 g. POCl3 heated gradually up to 100°, the mixture kept 5 min. at 110-15°, cooled, the residue in 50 ml. CHCl3 at 0° shaken with 40 ml. concentrated NH4OH, the CHCl3 layer passed through 16 ml. Al2O3, and the effluent concentrated gave 4.9 g. 6-chlorophenanthridine (III), needles, m. 116-17°; 3 g. I in 20 ml. CHCl3 treated dropwise with 4 g. SO2Cl2, the mixture refluxed 5 min., and the product treated as above gave 2.8 g. III, m. 116-17°. III (6 g.) in 6 ml. C6H6, 6 g. PhOH, and 6 g. K2CO3 heated 2 hrs. at 100°, cooled, 15 ml. 10% NaOH added, the product extracted with 30 ml. CHCl3, concentrated to 10 ml., and 10 ml. (Me2CH)2O added gave 7.1 g. 6-phenoxyphenanthridine (IV), columns, m. 116-17°. IV (1 g.) and 1.5 g. PhNH2 heated 2 hrs. at 180°, cooled, and 1 ml. AcOH and 5 ml. H2O added gave 0.7 g. II, m. 153-4° (MeOH).
IT 846-62-8, Phenanthridine, 6-anilino- (preparation of)
RN 846-62-8 CA
CN 6-Phenanthridinamine, N-phenyl- (9CI) (CA INDEX NAME)

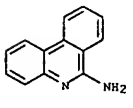


L8 ANSWER 60 OF 77 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 54:62618 CA
ORIGINAL REFERENCE NO.: 54:12077c-h
TITLE: Some derivatives of 5,6,7,8-tetrahydrophenanthridine
AUTHOR(S): Hollingsworth, B. L.; Petrow, V.
CORPORATE SOURCE: Univ. London
SOURCE: Journal of the Chemical Society, Abstracts (1960) 263-6
CODEN: JCSAAZ; ISSN: 0590-9791
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 54:62618
AB cf. C.A. 43, 1778g. Cyclohexanone (100 g.), 18 g. H2CO and 22 g. Et2NH.HCl refluxed 6 min., then the crude product refluxed 16 hrs. with 16.5 g. p-H2NC6H4CO2Et, 20.2 g. p-H2NC6H4CO2Et.HCl and 40 g. SnCl4.H2O, the mixture cooled, basified, extracted with Et2O and the extract in EtOH treated with picric acid gave Et 5,6,7,8-tetrahydrophenanthridine-3-carboxylate (I), m. 75°, as the picrate, m. 212-13°; saponification of I gave the acid, m. 312°, converted with POCl3-PCl5 to the acid chloride (II), and this to the amide (III), m. 250-2°. III (1 g.) added to an ice-cold solution of 1 g. Br in 12 ml. 10% KOH, the mixture kept 45 min. at 0°, 8 ml. 10% KOH added, the mixture heated 30 min. on a water bath, then chilled yielded 0.45 g. 3-amino-5,6,7,8-tetrahydrophenanthridine, m. 168-70° (benzamide m. 224-5°). II with NHEt2 in C6H6 gave the 3-diethylamino analog, m. 100-1°, and the 3-dimethylamino analog (IV), m. 95-6° (picrate m. 250-1°), was similarly prepared from N,N-dimethyl-p-phenylenediamine. 3-Methoxy-5,6,7,8-phenanthridine (3 g.) refluxed 2 hrs. with 15 ml. constant boiling HBr and worked up gave 2.5 g. 3-hydroxy analog of IV, m. 288-9° (picrate m. 221-3°; benzoate m. 138-9°). IV (4 g.), 15 ml. PhNEt2 and 4 g. NaNH2 heated 4 hrs. at 160°, the black precipitate taken up in 32% AcOH and basified yielded 9-amino-3-dimethylamino-5,6,7,8-tetrahydrophenanthridine, m. 185-7° (acetate salt m. 222-3°). 2-Methyl-5,6,7,8-tetrahydrophenanthridine, m. 57° (picrate m. 231-2°), was prepared from m-H2NC6H4Me and the 3-chloroanalog, m. 90° (10-oxide m. 169-70°; nitrate m. 152-3°), was prepared from p-ClC6H4NH2. 5,6,7,8-Tetrahydrophenanthridine (V) nitrate, m. 156-7°, (3.3 g.) added to 6 ml. H2SO4 and 4 ml. 30%, oleum at 0°, kept 30 min. at 0°, heated 1 hr. on a water bath, poured into H2O and neutralized precipitated the 4-nitro derivative of V, m. 119-20°, and this reduced and benzoylated gave the 4-benzamido analog, m. 149-50°. 2-Phenyliminomethylcyclohexanone (50 g.) refluxed 20 hrs. with 400 ml. HCO2H, the mixture concentrated, poured into aq NH3 and the base purified through the picrate gave 20% 2-anilinomethylcyclohexanone (VI), m. 88-9° (picrate m. 228-9°). VI (5 g.), 4 g. PhNH3Cl and 5 g. SnCl4 in 100 ml. alc. refluxed 8 hrs. gave 70% V, m. 63°.
IT 100949-91-5, Phenanthridine, 6-amino-2-dimethylamino-7,8,9,10-tetrahydro-
(preparation of)

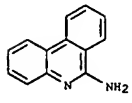
L8 ANSWER 60 OF 77 CA COPYRIGHT 2005 ACS on STN (Continued)
RN 100949-91-5 CA
CN Phenanthridine, 6-amino-2-dimethylamino-7,8,9,10-tetrahydro- (6CI) (CA INDEX NAME)



L8 ANSWER 61 OF 77 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 54:14675 CA
ORIGINAL REFERENCE NO.: 54:2893i,2894a-c
TITLE: Heats and entropies of ionization of some aromatic and N-heteroaromatic amines
AUTHOR(S): Elliott, J. J.; Mason, S. F.
CORPORATE SOURCE: Univ. Exeter, UK
SOURCE: Journal of the Chemical Society, Abstracts (1959) 2352-9
CODEN: JCSAAZ; ISSN: 0590-9791
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB The ionization consts. of a series of unsubstituted polycyclic aromatic amines were measured at 0 and 20° in 50% EtOH-H2O solution, and those of a series of N-heteroaromatic amines at 5 and 35° in H2O. Entropies and enthalpies of ionization were calculated The compds. studied were PhNH2; o-, m-, and p-NH2C6H4Ph; 2-aminofluorene; 1- and 2-naphthylamine; 1-, 2-, 3-, and 9-phenanthrylamine; 1-, 2-, and 9-anthrylamine; 3-aminopyrene; 2-, 3-, and 4-aminopyridine; 2-, 3-, 4-, 5-, 6-, 7-, and 8-aminoquinoline; 1-, 3-, 4-, 5-, 6-, 7-, and 8-aminoisoquinoline; 1-, 2-, 3-, 4-, and 5-aminoacridine; 6- and 9-aminophenanthridine; 2-amino-4-methyl-5,6-, 1'- and 4'-amino-5,6-, 3-amino-6,7-, and 2-amino-4-methyl-7,8-benzoquinoline; 8-amino-1,2-, and 8-amino-3,4-benzacridine. The variation in the ionization consts. of the aromatic amines is due equally to the entropy and the enthalpy factor, whereas the variation in the N-heteroaromatic series is due primarily to enthalpy changes. The dissociation entropies of the conjugate acids of the periaromatic amines are larger than those of the unhindered isomers, which in turn have larger values than those of the N-heteroaromatic amines. These results are discussed in relation to the solvation of the amine cations and the π-electron energy changes accompanying their dissociation
IT 832-68-8, Phenanthridine, 6-amino-
(ionization of)
RN 832-68-8 CA
CN 6-Phenanthridinamine (9CI) (CA INDEX NAME)



L8 ANSWER 62 OF 77 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 53:76177 CA
ORIGINAL REFERENCE NO.: 53:13779i,13780a-b
TITLE: The tautomerism of N-heteroaromatic amines
AUTHOR(S): Mason, S. F.
CORPORATE SOURCE: Univ. Exeter, UK
SOURCE: Journal of the Chemical Society, Abstracts (1959) 1281-8
CODEN: JCSAAZ; ISSN: 0590-9791
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB Infrared spectroscopy was used to study imine-amine tautomerism. The frequencies, extinction coeffs., and band half-widths of the absorption bands due to the N-H stretching vibrations of 23 primary and 7 secondary tri- and tetracyclic N-heteroaromatic amines and imines in dilute CCl4 solution were measured in the 3-μ region. The imines absorbed weakly near 3300 cm.-1; the amines absorbed 5 to 10 times as intensely at slightly higher frequencies. These spectral differences were used to show that most of the tetracyclic and all of the tricyclic amines studied exist primarily as the amino tautomer; an exception was 5-amino-2,3-benzacridine which exists mostly in the imino form. A review of ultraviolet data and an examination of the ionization constant for 5-aminoacridine concurred with the infrared finding that this compound exists in the amino form.
IT 832-68-8, Phenanthridine, 6-amino-
(spectra of, tautomerism and)
RN 832-68-8 CA
CN 6-Phenanthridinamine (9CI) (CA INDEX NAME)

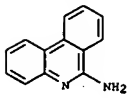


L8 ANSWER 63 OF 77 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 52:82602 CA
ORIGINAL REFERENCE NO.: 52:14621f-i
TITLE: Tautomerism and steric properties of 9-substituted phenanthridines
AUTHOR(S): Reese, C. B.
CORPORATE SOURCE: Univ. Chem. Lab., Cambridge, UK
SOURCE: Journal of the Chemical Society, Abstracts (1958) 895-9
CODEN: JCSAAZ; ISSN: 0590-9791
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB The amino form of 9-aminophenanthridine (I) (C.A.: 6-aminophenanthridine) was found to predominate in aqueous-alc. solution The tautomeric equilibrium of the isomeric 5-aminoacridine is considered in comparison. The ultraviolet absorption spectra of the MeI salts of I, 9-methylamino- (II), and 9-dimethylaminophenanthridine (III) were examined Phenanthridone (IV) was shown to adopt the lactam form in alc. 9-Chlorophenanthridine (V) (3 g.) and MeOH saturated with 8 cc. NH3 at 0°, heated 5 hrs. at 180°, the solvent removed, the residue extracted with H2SO4, and the extract neutralized gave 1.6 g. I, sublimed at 140°/0.5 mm., m. 193-5°. I (0.31 g.) and 1 cc. MeI heated 4 hrs. at 125° gave I.MeI (VI), m. 257° (MeOH), in quant. yield. VI (0.25 g.) suspended in 50 cc. CHCl3, shaken with 10 cc. 3N aqueous NaOH until the turbidity in the aqueous layer disappeared, the CHCl3 layer dried, the solvent removed, and the brown gum azeotropically distilled gave 0.065 g. crude 9,10-dihydro-9-imino-10-methylphenanthridine, which, purified by "cold finger" distillation at 110°/0.5 mm., m. 92°. II prepared by a known method m. 187-8°. V (1 g.) heated 2 hrs. at 100° with 2 g. pure anhydrous NHMe2, the excess amine evaporated, the residue extracted with C6H6, and the solvent removed gave a gum in quant. yield; recrystn. yielded III which b0.5 110°, m. 60°. II (0.31 g.) quaternized with excess MeI as above gave the methiodide hemihydrate, m. 223-4° with darkening and effervescence. Similarly, III gave the methiodide, m. 222° (decomposition). V (0.21 g.) in 30 cc. anhydrous MeOH treated under reflux 0.5 hr. with NaOMe (from 0.1 g. Na) and 8 cc. MeOH, the solvents removed, the C6H6 extract evaporated, and the residue subjected to a "cold finger" distillation gave 9-methoxyphenanthridine (VII), b1.0 108°, m. 52°. The curve for IV was like that of 10-methylphenanthridone but quite unlike VII. The spectral curves for many of the above compds. are given.

IT 832-68-8, Phenanthridine, 6-amino-
(preparation of)
RN 832-68-8 CA
CN 6-Phenanthridinamine (9CI) (CA INDEX NAME)

L8 ANSWER 63 OF 77 CA COPYRIGHT 2005 ACS on STN (Continued)



L8 ANSWER 64 OF 77 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 52:55935 CA
ORIGINAL REFERENCE NO.: 52:10095e-i,10096a-i,10097a-g
TITLE: Aminoisoquinolines, -cinnolines, and -quinazolines. (A) The basic strengths and ultraviolet absorption spectra. (B) Infrared spectra
AUTHOR(S): Osborn, A. R.; Schofield, K.; Short, L. N.
CORPORATE SOURCE: Washington Singer Labs., Exeter, UK
SOURCE: Journal of the Chemical Society, Abstracts (1956) 4191-206
CODEN: JCSAAZ; ISSN: 0590-9791
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB cf. following abstract Potentiometric titrations in aqueous solution at 20° with HCl gave the following pKa values. Isoquinolines: unsubstituted (I), 5.40; 3-NH2 (Ia), 5.05; 4-NH2 (Ib), 6.28; 5-NH2 (Ic), 5.59; 6-NH2 (Id), 7.17; 7-NH2 (Ie), 6.20; 8-NH2 (If), 6.06. Cinnolines: unsubstituted (II), 2.29; 3-NH2 (IIa), 3.70; 4-NH2 (IIb), 6.85; 5-NH2 (IIc), 2.70; 6-NH2 (IId), 5.04; 7-NH2 (IIe), 4.85; 8-NH2 (IIf), 3.68. Quinazolines: unsubstituted (III), 3.51; 2-NH2 (IIIa), 4.82; 4-NH2 (IIIb), 5.85; 5-NH2 (IIIc), 3.57; 6-NH2 (IIId), 3.29; 7-NH2 (IIIe), 4.60; 8-NH2 (IIIf), 2.81. In addition pKa values based on calcns. from ultraviolet extinction curves were determined for phenanthridine 4.52, its 6-NH2 derivative 6.88, and 6,7-benzoquinazoline (IV) .apprx. 5.2. Ultraviolet absorption data for the above bases and their cations in buffered aqueous solns. and of the methochlorides of I, II, and III in H2O were given. I, II, and III showed the 3 main bands characteristic of electronic transitions parallel to the long, short, and long axes of bicyclic systems, and the effect of the position of the NH2 substituent could be correlated fairly well with the shifts of the bands noted in the spectra of their NH2 derivs. II in cyclohexane showed an addnl. low-intensity, longer wavelength (390 mμ) band of an n → π transition which disappeared in water or acid. The bathochromic shift shown in the spectra of the aminoisoquinolines on conversion to the cations indicated that, as with I, the monocations carry the proton on the ring N. Study of the ΔpKa values (relative to I) showed values below 1 for Ib, Ic, and Ie, in which there is no possibility of addnl. ionic resonance in the cations, and above 1 for the 1-NH2 derivative of I and Id, for which addnl. forms are possible, and a neg. value for Ia, which is clearly not increased in stability by a possible o-quinonoid resonance form (see the following abstract for If). The bathochromic shifts in the spectra of the aminocinnolines on cation formation again indicated that proton attachment is to the ring N. By analogies to the quinoline and isoquinoline series, ΔpKa values indicated that N1 is the predominant basic center in IIb, IIe, and probably IIc, while N2 is the basic center for IId and IIf (the spectra of If and IIf are similar). From the values of ΔpKa for IIa, the basic center is considered to be N2, although it contrasts strongly with Ia. Cationization of III caused a marked hypsochromic shift in contrast to the more usual slight bathochromic shift for other heterocyclic bases, and

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AB some modification of the aromatic system, possibly a 3,4-hydration, is assumed. Ultraviolet studies on cation formation of the aminoquinazolines indicated no hydration for IIIa and IIIb (similar to 2- and 4-aminoquinoline), IIIc, IIIe, and IIIf, while IIId is presumably hydrated. Considering the change on cationization of III and the increased base strength of 3,4-dihydroquinazolines relative to the quinazolines, choice of a basic center by correlation with ΔpKa values is difficult, although N1 seems to be favored for IIIb and definite for IIIe. Quinoxaline and its 6-NH2 deriv. also showed the usual bathochromic shift on cation formation, while the 5-NH2 deriv. seemed to take up the first proton on its NH2 group. Infrared N-H bond stretching frequencies and force constants, indicative of the amt. of interaction of the NH2 group with the ring and the electron density at the ring N, were given for Ia-f, IIa-f, IIIa-f, 2-, 4-, and 5-aminopyrimidines, and 5-aminoquinoline in CCl4, CHCl3, and pyridine (some compds.); the effects of electromeric interaction where possible, the lack of interaction between N1 and a C-5 NH2 group, the effect of 2 ring N atoms adjacent to the NH2 group and of intramolecular H-bonding were noted. 1,3-Dichloroisoquinoline (0.5 g.), 25 cc. MeOH, 0.4 g. KOH, and 3 cc. Raney Ni shaken with H, the MeOH evapd., and the Et2O ext. of the residue treated with picric acid in Et2O gave I picrate, m. 225-6°; 1,3-dibromoisoquinoline (V) behaved similarly. Homophthalimide (5 g.) and 50 cc. PBr3 refluxed 5 hrs., the PBr3 evapd. in vacuo, and the residue treated with alkali gave 3.4 g. V, m. 147-7.5° (MeOH). V (3 g.) was converted to 1.75 g. 3-bromoisoquinoline (VI), m. 63-4° (aq. MeOH). 3-Chloroisoquinoline (8.8 g.), 100 cc. concd. NH4OH, and 1 g. CuSO4 heated 30 hrs. at 140° in an autoclave, made strongly basic, and extd. with CHCl3 gave 5.3 g. Ia, m. 176-7° (C6H6), similarly prepd. from VI. Ib m. 108-9.5° (C6H6-cyclohexane). 5-Nitroisoquinoline (20 g.), 500 cc. MeOH, and 2 g. 5% Pd-C hydrogenated 2 hrs., evapd., and the residue crystd. from CHCl3-petr. ether gave 93% Ic, m. 129.5-30.5° (C6H6-cyclohexane). m-MeOC6H4CHO (35.5 g.), 18 g. MeNO2, 125 cc. HOAc, and 12.5 g. NH4OAc refluxed 2 hrs. and poured into H2O gave 27 g. m-MeOC6H4CH:CHNO2, m. 91-2° (C6H6), which was not reduced satisfactorily. 1,2,3,4-Tetrahydro-6-methoxyisoquinoline (2.42 g.) and 0.8 g. 30% Pd-C heated 0.25 hr. at 180-90° in a stream of N, extd. with Et2O, the 2.1 g. oily product treated with 3 g. picric acid in 10 cc. Me2CO, the 2.9 g. picrate decompd. with aq. LiOH, extd. with Et2O, the 1.03 g. product refluxed 2 hrs. with 25 cc. concd. HBr, evapd. in vacuo, dissolved in 10 cc. H2O, and treated with aq. Na2CO3 gave 0.85 g. 6-hydroxyisoquinoline (VII), m. 220° (decompn.); dehydrogenation with Raney Ni in naphthalene was unsuccessful. Id, m. 211-12° (C6H6), was prepd. from VII. 1,3-Dihydroxy-7-nitroisoquinoline (VIII) (52 g.), m. 291° (decompn.), was prepd. from 56 g. 4-nitrohomophthalic acid in o-C6H4Cl2. VIII (2 g.) and 20 cc. POCl3 heated 4 hrs. on the steam bath, decompd. with ice, and brought to pH 10 gave 1.18 g. 1,3-dichloro-7-nitroisoquinoline, m. 185° (decompn.) (HOAc), but the reaction was not reproducible. 7-Hydroxyisoquinoline (1.25 g.), 4 cc. NH4SO3 (concd. NH4OH satd. with SO2), and 20 cc. concd. NH4OH 16 hrs. at 140-50° gave 1.1 g. Ie, m. 203-5° (C6H6) after sublimation at 150°/0.3 mm. Ic (4.8 g.) in 12 cc. concd. HBr and 13 cc. H2O diazotized at 0° with 2.3 g. NaNO2 in 15 cc. H2O, added to 5.8 g. CuBr in 48 cc. HBr at 75°, and let stand 24 hrs. gave 5.1 g.

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5-bromoisoquinoline (IX), m. 82-4° (petr. ether). KNO3 (2.4 g.) in 20 cc. concd. H2SO4 added during 5 min. to 4.15 g. IX in 24 cc. concd. H2SO4, the mixt. let stand 1 hr. at room temp., poured on ice, and made alk. with NH4OH gave 5.05 g. 5-bromo-8-nitroisoquinoline (X), m. 139-41° (MeOH). 5-Chloro-8-nitroisoquinoline (2 g.) and 12 g. NH4OAc added to 2 g. 6% Pd-CaCO3 in abs. MeOH (previously shaken with H), hydrogenated 1 hr., the filtered soln. acidified with concd. HCl, the MeOH evapd. in vacuo, the residue in H2O made alk. with satd. Na2CO3, and extd. with CHCl3 gave 1.02 g. If, m. 171-2° (EtOAc); use of NaOAc in the reduction gave lower yields of If while reduction with Pd-C in MeOH in the presence of NaOAc gave 8-amino-5-chloroisoquinoline, from which the Cl was not removed on Raney Ni hydrogenation in alk. soln.; hydrogenation of X in MeOH over Pd-CaCO3 gave colored intermediate products, while reduction of X in the presence of KOH gave a small yield of If. 2-Chloroquinazoline (0.5 g.) added slowly to 0.4 g. KOH in 5 g. PhOH, the mixt. heated 3 hrs. at 70°, and made alk. gave 0.58 g. 2-phenoxyquinazoline (XI), m. 124-6° (petr. ether). XI (0.5 g.) and 5 g. NH4OAc heated 2 hrs. at 170-80° and treated with H2O and 2N NaOH gave 0.35 g. IIIa, m. 200° (EtOH). IIIb m. 271-2° (EtOH). 6,2-O2N(H2N)C6H3CO2H (14.84 g.) and 29.4 cc. HCONH2 4.5 hrs. at 155-60° gave 12.2 g. 4-hydroxy-5-nitroquinazoline (XII), m. 252-6° (H2O). XII (7 g.) and POCl3 gave 5.17 g. 4-chloro-5-nitroquinazoline (XIII), m. 142° after sublimation at 140°/0.5 mm. Resublimed XIII (1 g.) in 150 cc. dry MeOCH2CH2OH and 0.5 g. 6% Pd-CaCO3 hydrogenated 0.5 hr., evapd., oxidized with K3Fe(CN)6, and the product chromatographed gave 0.265 g. IIIc, m. 195-6.5° (C6H6) after sublimation at 160°/1 mm. IIId, m. 213-14° (C6H6), IIIe, m. 190-1° (C6H6) after sublimation at 160°/0.5 mm., and IIIf, m. 150-1° after sublimation at 120°/0.5 mm., were prepd. similarly by reduction at atm. pressure with 6% Pd-C. 1-Chloro-7-methoxyphthalazine (XIV) (7.4 g.), m. 142° (decompn.), was obtained by refluxing 8.8 g. 1-OH compd. 0.5 hr. with 40 cc. POCl3. XIV (0.5 g.), 0.2 g. red P, and 5 cc. HI refluxed 1 hr., dild. with 5 cc. H2O, evapd. in vacuo, and the residue in 5 cc. H2O adjusted to pH 7 with NH4OH gave 0.3 g. 6-hydroxyphthalazine-0.5H2O, m. 300° (decompn.) (H2O), which was not converted successfully to the 6-NH2 compd. XIV refluxed with HBr gave 4,6-dihydroxyphthalazine, m. 310° (decompn.) (H2O). 3,2-H2NC10H6CO 2H (10 g.) was converted to 8.5 g. 4-hydroxy-6,7-benzoquinazoline (XV), m. 278° (H2O). XV (1.3 g.) and 20 cc. POCl3 refluxed 2 hrs. gave 0.98 g. 4-chloro-6,7-benzoquinazoline (XVI), m. 176-8° after sublimation at 160°/0.1 mm. XVI (0.4 g.) in 50 cc. MeOCH2CH2OH hydrogenated 1.5 hrs. over 0.5 g. 8% Pd-CaCO3 and the product in H2O oxidized with 1.4 g. K3Fe(CN)6 gave 0.19 g. IV, m. 163-5° (cyclohexane) after sublimation. XVI (0.23 g.) and 25 cc. satd. NH3-MeOH refluxed 2 hrs. gave 4-amino-6,7-benzoquinazoline, m. 365° (decompn.) (EtOH) after repeated sublimation. XVI (2.1 g.) in 100 cc. warm C6H6 added to 2 equivs. NaCH(CO2Et)2 in 100 cc. C6H6, refluxed 3 hrs., let stand

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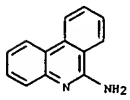
overnight, poured into H2O, the org. layer evapd., and the residue crystd. from EtOH gave 2.29 g. di-Et 6,7-benzoquinazol-4-ylmalonate (XVII), m. 172-5°. XVII (1.5 g.), 0.6 g. KOH, and 60 cc. MeOH refluxed 3 hrs. gave 0.58 g. 6,7-benzoquinazol-4-ylacetate, m. 207-9° (MeOH), hydrolyzed with boiling aq. NaOH to traces of 4-methyl-6,7-benzoquinazoline-1.5H2O, m. 124-6° (petr. ether). I (5 g.), 10 cc. MeI, and MeOH refluxed 2 hrs. gave I methiodide, m. 160-1.5° (EtOH), which was shaken with 50 cc. H2O and excess freshly pptd. AgCl for 12 hrs., filtered, the filtrate evapd., and I methochloride crystd. under anhyd. conditions from EtOH-Et2O. Quinoline methochloride, the very deliquescent II methochloride-0.5H2O, and 4-methylcinnoline methochloride-H2O were prepd. similarly.

IT **832-68-8**, Phenanthridine, 6-amino-
(basicity and spectrum of)

RN 832-68-8 CA

CN 6-Phenanthridinamine (9CI) (CA INDEX NAME)



L8 ANSWER 65 OF 77 CA COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 50:69424 CA

ORIGINAL REFERENCE NO.: 50:13019c-i,13020a-e

TITLE: New trypanocides. I. Quaternary salts derived from 2,7-diaminophenanthridine and the attempted preparation of quaternary salts from 2,7-diamino-9-anilinophenanthridine

AUTHOR(S): Davis, M.

CORPORATE SOURCE: May & Baker Ltd., Dagenham, Essex, UK

SOURCE: Journal of the Chemical Society, Abstracts (1956) 337-43
CODEN: JCSAAZ; ISSN: 0590-9791

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB Salts of 2,7-diamino-(I) and 2,7-bis(ethoxycarbonylamino)-10-methylphenanthridine (II) were prepared by 2 routes. 2,7-Diamino-9-anilino-(III) and -9-p-aminoanilinophenanthridine (IV) were prepared from 9-chloro-2,7-dinitrophenanthridine (V). Attempts to convert III and IV into quaternary derivs. were unsuccessful. 2,7-Diaminofluorenone (31.3 g.) in concentrated H2SO4 cooled to -30° was treated during 1.25 h. below 0° with 21.8 g. NaN3 in H2O, 75 mL. H2O added during the next 0.75 h., and the solution poured on ice and aqueous NH3 to yield 26 g. 2,7-diaminophenanthridone (VI), m. 310-12° (decomposition) (from PhNO2). Heating 1 g. VI with MeI in MeOH 24 h. at 115° gave 98% 2,7-bisdimethylaminophenanthridine-2-MeI.2H2O (VII), m. 330-4° (decomposition), which on drying gave the monohydrate, and finally the anhydrous salt, λ0.1N HCl 336, 325, and 260 mμ (ε 8200, 9700, and 23,300), λinfl. 269 mμ (ε 14,200). VI (24.3 g.), 25.8 mL. ClCO2Et, 43 mL. PhNEt2, and 700 mL. EtOH refluxed 3 h. formed 33.6 g. 2,7-di(ethoxycarbonylamino)phenanthridone (VIII), prisms, m. above 360° (from dioxane). VIII (11.2 g.) refluxed 0.5 h. with 55 mL. POCl3 gave 7.95 g. 9-chloro-2,7-bis(ethoxycarbonylamino)phenanthridine (IX), m. 252-4° (decomposition) (from EtOH). 2,7-Bis(ethoxycarbonylamino)-9-methylphenanthridine (10 g.) and 3.05 g. SeO2 refluxed 7 h. in 400 mL. dioxane and 10 mL. H2O yielded 7.45 g. 2,7-bis(ethoxycarbonylamino)-9-formylphenanthridine (X), m. 250-62° (decomposition). X (12 g.) heated at 50-5° in 157 mL. C5H5N, 3.7 g. KMnO4 in H2O added during 1.5 h., after a further 1.5 h. at 50-5° the mixture was refluxed and filtered, and the residue extracted with hot C5H5N and K2CO3 solution The C5H5N exts. were combined with the original filtrate, concentrated to 150 mL. and the carbonate extract added, the mixture refluxed, and filtered. The residue after further extraction with K2CO3 solution was 2.85 g. unchanged X. The combined exts. upon acidification gave 5.3 g. 2,7-bis(ethoxycarbonylamino)phenanthridine-9-carboxylic acid (XI). XI (5 g.) in 25 mL. PhNO2 refluxed 2 h. gave 3.2 g. 2,7-bis(ethoxycarbonylamino)phenanthridine (XII), m. 250-3° (decomposition) (from alc.). IX (4 g.) suspended in 400 mL. hot alc. containing 1 g. KOH and Raney Ni was shaken with H, fresh catalyst added, and the suspension reheated gave 2.1 g. XII. On one occasion when 4 g. of IX was similarly reduced under pressure 2.85 g. of 2,7-bis(ethoxycarbonylamino)-9,10-dihydrophenanthridine was obtained, m. 192-4°; Ac derivative, m. 230-2°. XII (0.5 g.) heated 0.5 h. at 160° in concentrated H2SO4 and H2O gave 2,7-diaminophenanthridine, m. 208-10° (decomposition). XII

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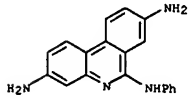
(3.2 g.) in PhNO2 treated 1 min. at 150° with 3.2 mL. Me2SO4 gave 4.15 g. of the Me methosulfate (XIII) of II as orange needles, decomp. above 280° from alc. (green fluorescence). XIII with KI in H2O gave the methiodide (XIV) yellow needles, decomp. above 260° (from alc.). XIV was also obtained from the original base with MeI-MeOH. XIII (4.15 g.) heated 45 min. at 140° in H2SO4-H2O yielded after treatment with KI 2.75 g. of the iodide (XV) of I. XV was similarly prepd. from XIV as red needles, m. 288-90° (decompn.). Refluxing an aq. soln. of XV with freshly prepd. AgCl gave the corresponding chloride, red prisms, m. 278-80° (decompn.). V (2 g.) and 9 mL. PhNH2 refluxed 1 h. gave 2.2 g. 9-anilino-2,7-dinitrophenanthridine (XVI), orange prisms, m. 316-18°. V similarly afforded 93% 2,7-dinitro-9-p-nitroanilinophenanthridine (XVII), decomp. 350-60° (from PhNO2); Ac deriv., decomp. 300-4°. XVI (2.2 g.) refluxed 0.5 h. with 20 g. SnCl2.2H2O in 20 mL. concd. HCl gave 1.45 g. III as yellow plates, m. 225-6° (decompn.); hydriodide, orange needles, m. 224-6° (decompn.); tri-Ac deriv. (XVIII), m. 300-4° (from Et2O-C5H5N). XVII similarly yielded 90% IV as yellow plates, m. 244-5° (decompn.); tri-Ac deriv. (XIX), m. 328-9° (decompn.); tetra-Ac deriv. (XX), decomp. 360°. IV (0.31 g.) in alc. refluxed 2 h. at 100° with 0.75 g. PhNEt2 and 0.55 g. ClCO2Et gave 2,7-bis(ethoxycarbonylamino)-9-p-ethoxycarbonylaminoanilinophenanthridine-HCl.H2O (XXI), m. 211-13° (decompn.); free base, m. 238-42° (from alc.). XVIII (0.6 g.), excess MeI, and MeOH refluxed 18 h. and left 3 days gave 0.63 g. of a salt, C26H25O3N4I (XXII), yellow plates, m. 330-40° (decompn.). XXII hydrolyzed with concd. HCl caused I to evolve and gave III, m. 224-6° (decompn.). XVIII (0.4 g.) similarly treated in a sealed tube 18 h. at 110° gave VII. IV (0.35 g.) with MeI-MeOH at 115° gave 0.25 g. VII. VII was also obtained from XIX at 140°. XX was recovered unchanged from refluxing MeI-MeOH after 20 h. At 110° VII was formed. XXII (0.53 g.) refluxed 13 h. with 0.05 g. Na2CO3 and excess MeI in alc. yielded 2,7-bis(ethoxycarbonylamino)-9-(N-methyl-p-ethoxycarbonylaminoanilino)-phenanthridine-HI, m. 250-5° (decompn.) (from Me2COEt2O); the base, amorphous, m. 210-20° (decompn.) (from aq. alc.). V (0.25 g.) and 0.1 g. PtO2 in 50 mL. dioxane when shaken with H gave an uptake of 160 mL. in 0.5 h. and the residue yielded the diamino chloro compd., yellow prisms, decomp. above 200° (from Me2CO-C6H6), sol. in dil. HCl and pptd. unchanged by alkali. The chloride of I was inactive against Trypanosoma rhodesiense and was effective, but not curative, against T. Congolese. XIII, XXI, and IV hydrochloride were inactive against both organisms.

IT **666236-95-9**, Phenanthridine, 3,8-diamino-6-anilino-
(and derivs.)

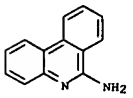
RN 666236-95-9 CA

CN Phenanthridine, 3,8-diamino-6-anilino- (5CI) (CA INDEX NAME)

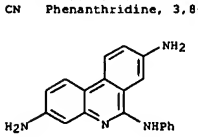


L8 ANSWER 65 OF 77 CA COPYRIGHT 2005 ACS on STN (Continued)

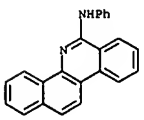
L8 ANSWER 66 OF 77 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 50:13544 CA
ORIGINAL REFERENCE NO.: 50:2841i,2842a
TITLE: Chemical constitution and antituberculous activity. III. Heterocyclic bases
AUTHOR(S): Cymerman-Craig, J.; Rubbo, S. D.; Loder, J. W.; Pierson, Barbara J.
CORPORATE SOURCE: Univ. Sydney, Australia
SOURCE: British Journal of Experimental Pathology (1955), 36, 261-7
CODEN: BJEPA5; ISSN: 0007-1021
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB Pyridines, quinolines, acridines, phenanthridines, benzacridines, dibenzacridines, nicotinamides, nicotinamidines, and benzimidazoles were tested for antituberculous activity, and those containing a primary NH2 were investigated in detail. Activity is proportional to the planar surface area of the mol. and by means of this factor, combined with those described in the previous paper, a 2000-fold increase of activity was accomplished. Marked specificity of antituberculous action was present.
IT 832-68-8, Phenanthridine, 6-amino-
(antitubercular activity of)
RN 832-68-8 CA
CN 6-Phenanthridinamine (9CI) (CA INDEX NAME)



L8 ANSWER 67 OF 77 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 49:54045 CA
ORIGINAL REFERENCE NO.: 49:10438a-e
TITLE: Properties of a small bacteriophage and the action of some compounds on it
AUTHOR(S): Mills, R. F. N.
CORPORATE SOURCE: Boots Pure Drug Co., Ltd., Nottingham, UK
SOURCE: Journal of General Microbiology (1955), 12, 172-9
CODEN: JGMIAN; ISSN: 0022-1287
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB Study of the multiplication of phage S13 showed that a latent period of 20 min. existed when Escherichia coli was the host, and intracellular multiplication was only detected at the end of the latent period. Photoreactivation of phage inactivated by UV light was observed Of 1600 chemical compds. tested for ability to inhibit phage multiplication without affecting the host cells, only the following 13 were found worthy of further study: 4,4'-di-2-imidazolin-2-ylstilbene dihydrochloride monohydrate (I), 2-hydroxy-4,4'-stilbenedicarboxamidine dihydrochloride dihydrate, phenylguanidine, 1,2-bis(4'-amidino-4-biphenylyloxy)ethane dihydrochloride, 1,4-bis(4'-amidino-4-biphenylyloxy)butane dihydrochloride, bis(p-picolinamidophenyl) ether, bis[p-[(p-methoxyphenyl)amidino]phenyl] ether, 6-(p-aminoanilino)phenanthridine, 3,8-diamino-6-anilinophenanthridine, 3,8-di-2-imidazolin-2-yl-6-phenylphenanthridine trihydrochloride dihydrate (II), 3,8-diamino-5-methyl-6-p-tolylphenanthridinium bromide, 3,8-diamino-5,6-dimethylphenanthridinium bromide (III), and 2,4,5,6-tetraaminopyrimidine sulfate monohydrate. Further study of the activity of I showed that multiplication early and late in the latent period was inhibited. When the 13 compds. were tested for inhibition of multiplication of T1 E. coli phage only I, II, and III inhibited phage multiplication. I had previously been reported to inhibit multiplication of Pseudomonas aeruginosa phage (Dickinson and Codd, C.A. 46, 10295d).
IT 666236-95-9, Phenanthridine, 3,8-diamino-6-anilino-
(effect of bacteriophages)
RN 666236-95-9 CA
CN Phenanthridine, 3,8-diamino-6-anilino- (5CI) (CA INDEX NAME)



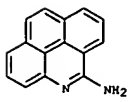
L8 ANSWER 68 OF 77 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 49:46284 CA
ORIGINAL REFERENCE NO.: 49:8969b-f
TITLE: Polynuclear heterocyclic systems. VIII. Synthetic applications of the Schmidt reaction
AUTHOR(S): Badger, G. M.; Seidler, J. H.
CORPORATE SOURCE: Univ. Adelaide
SOURCE: Journal of the Chemical Society, Abstracts (1954) 2329-33
CODEN: JCSAAZ; ISSN: 0590-9791
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 49:46284
AB cf. C.A. 48, 11413e. The Schmidt reaction with 5,6-chrysenequinone gives 2-(o-carbamoylphenyl)-1-naphthoic acid (I), while the Beckmann rearrangement of chrysenequinone monoxime forms I and the isomeric 2-o-carboxyphenyl-1-naphthamide (II). By treatment with NaN3 in H2SO4 I and II were converted into 1,2-benzophenanthridone (III) and 7,8-benzophenanthridone (IV), resp. III (2 g.) was refluxed 4 hours with 18 cc. POCl3 and 0.6 cc. PhNMe2, excess POCl3 removed, residue poured into cold H2O and extracted with C6H6, evaporation of the C6H6 and recrystn. from EtOH gave 90% 9-chloro-1,2-benzophenanthridine (V), m. 156.5°, sublimes at 120° at 5 + 10-5 mm. V and PhNH2 gave 2-anilino-1,2-benzophenanthridine, m. 152°. 1,2-Benzophenanthridine (VI) was obtained by (a) hydrogenation of V in alc. KOH over Raney Ni (86% yield); (b) treatment of III with LiAlH4 in dioxane (giving presumably the CH2 analog, m. 213°), followed by dehydrogenation with Pt on asbestos in cymene (95% yield); or (c) reduction of V with LiAlH4 in dioxane (100% yield). IV (1 g.) and POCl3 gave, similarly to the above, 0.83 g. 9-chloro-7,8-benzophenanthridine (VII), m. 163°. VII with EtOH and POCl3 or NaOEt gave 9-ethoxy-7,8-benzophenanthridine, m. 125.5°. VII was changed back to IV by refluxing in EtOH or alc. HCl, although V was unaffected by these treatments. VII with PhNH2 gave 9-anilino-7,8-benzophenanthridine, m. 155°. VII was converted to 7,8-benzophenanthridine by methods similar to those used for converting V to VI.
IT 853914-25-7, Benzo[c]phenanthridine, 6-anilino-
(preparation of)
RN 853914-25-7 CA
CN Benzo[c]phenanthridine, 6-anilino- (5CI) (CA INDEX NAME)



L8 ANSWER 69 OF 77 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 48:7226 CA
ORIGINAL REFERENCE NO.: 48:1359f-i,1360a-b
TITLE: Synthesis of 1-azapyrene and phenanthrylene-4,5-methane
AUTHOR(S): Medenwald, Hans
CORPORATE SOURCE: Tech. Hochschule, Karlsruhe, Germany
SOURCE: Chemische Berichte (1953), 86, 287-93
CODEN: CHBEAM; ISSN: 0009-2940
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB Heating 25 g. phenanthrene-4-aldehyde-5-carboxylic acid (I) in 250 cc. 2N NaOH and 200 cc. H2O with a saturated aqueous solution of 8.5 g. H2NOH.HCl 1 hr. at 90-100° gives 26.5 g. 4-oxime which, treated with 200 cc. SOCl2, gives 70% 4-cyanophenanthrene-5-carboxylic acid chloride (II), stout crystals, m. 220°. Slowly heating 26.5 g. II in 110 cc. H2O and 250 cc. concentrated H2SO4, finally 1.5 hrs. at 125-40° under reflux, and diluting with H2O give 21 g. phenanthrene-4,5-dicarboxylic acid (III), m. 260° with loss of H2O. Heating 3-4 g. III at 260-90° gives 70-5% phenanthrene-4,5-dicarboxylic anhydride (IV), needles, m. 260°. Adding 15 cc. concentrated NH4OH to 3.4 g. IV in 100 cc. boiling dioxane gives 87% NH4 salt of phenanthrene-4-carboxylic acid-5-carbamide (V) which, decomposed with 2N HCl, gives V, m. 195-235°, probably with the formation of the 4,5-imide. Heating 1.55 g. V in 40 cc. 2N NaOH with 17 cc. NaOBr solution (prepared from 3.5 g. NaOH and 4 g. Br in 50 cc. H2O), adding 60 cc. H2O, heating the mixture 0.75 hr. on a water bath, and saturating it with SO2 give 50% 2-oxo-1,2-dihydro-1-azapyrene [5(4H)-thebenidinone] (VI), m. 340°. Adding 1.8 g. NaN3 to 6 g. I in 26 cc. concentrated H2SO4 overlayered with 100 cc. CHCl3, diluting the mixture with ice to 400 cc., distilling off the CHCl3, and refluxing the residue 15 min. give 25% VI. Heating the Ba salt from 5 g. III at 380-415°/12 mm. gives 47% phenanthrylene-4,5-ketone (4H-cyclopenta[def]phenanthen-4-one) (VII), long yellow needles, m. 170° (oxime, light yellow needles, m. 252°). Heating 0.5 g. VI with 5 g. Zn dust with the free flame and purifying the reaction product by sublimation give 6% 1-azapyrene, m. 157-9°. Heating 6.5 g. II with 3 g. NaN3 in 125 g. moist dioxane 3 hrs. at 90-100°, evaporating the mixture with 10 cc. concentrated HCl on a water bath, and making the residue in 250 cc. H2O alkaline with 2N NaOH give 75% 2-imino-1,2-dihydro-1-azapyrene (VIII), needles, m. 237° (Ac derivative, prepared by boiling with Ac2O, long needles, m. 238°). VIII in dioxane or AcOH fluoresces blue-violet. Refluxing 220 mg. VII with 0.3 g. N2H4.H2O, 0.2 g. KOH, and 4 cc. (CH2OH)2 10-15 hrs. gives 60% phenanthrylene-4,5-methane (4H-cyclopenta[def]phenanthrene), leaflets, m. 114-15°. Refluxing 3.2 g. II in 100 cc. dioxane with 10 cc. concentrated HCl 1.5 hrs. gives 70% phenanthrene-4,5-dicarboximide (IX), m. 240°, which is also obtained in 90% yield when equal amts. of urea and IV are heated at 180°. Treating IX in dioxane with CH2N2 in ether at 25-30° gives the N-Me derivative, needles, m. 176°. The infrared absorption curves of VI and IX are given.

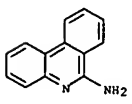
L8 ANSWER 69 OF 77 CA COPYRIGHT 2005 ACS on STN (Continued)
IT 857750-48-2, Thebenidine, 4,5-dihydro-5-imino- (preparation of)
RN 857750-48-2 CA
CN Thebenidine, 4,5-dihydro-5-imino- (5CI) (CA INDEX NAME)



L8 ANSWER 70 OF 77 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 47:57463 CA
ORIGINAL REFERENCE NO.: 47:9724b-f
TITLE: Lipoid-water partition coefficients of some aromatic bases
AUTHOR(S): Cymerman, J.; Diamantis, A. A.
CORPORATE SOURCE: Univ. Sydney, Australia
SOURCE: Journal of the Chemical Society, Abstracts (1953) 1619-21
CODEN: JCSAAZ; ISSN: 0590-9791
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB Apparent partition consts., k, between liquid paraffin and aqueous phosphate buffer (pH 7.2) were determined at 20° by spectrophotometric examination of the aqueous phase for a number of aromatic bases exhibiting tuberculostatic activity. Values of k (given as B0/[Bω + BH+], where B0 and Bω are concns. of undissocd. base) are listed for the following hydrochlorides: p-2-pyridylaniline (2HCl), m. 310-13° decompose, 0.47; o-aminophenol, <1, p-aminophenol, <1, p-piperidinoaniline (2HCl), 1.28; p-toluidine, 2.00; p-chloroaniline, 3.14; 2-naphthylamine, 9.5; 1-naphthylamine, 9.7; 2-aminofluorene (m.p. 321-2°, decompose, from MeOH), 57; 2-aminochrysene (m.p. 274-5°, decompose, from MeOH), insol. in H2O; 9-aminophenanthrene (m.p. 278-80°), 72; 4-aminoquinoline (m. 308°, from MeOH, anhydrous after drying at 120°), 0.02; 5-aminoacridine, 0.15; 5-amino-1-methylacridine 0.19; 5-amino-1,2-benzacridine (m.p. 380°, decompose, from MeOH), 4.90; 9-aminophenanthridine (m.p. 309°), 3.10; 9-amino-3-methylphenanthridine (m.p. 349-50°), 8.30; 9-amino-1,3-dimethylphenanthridine (m.p. 372°, decompose), 47.0; N'-p-biphenylyl-N,N-diethylethylenediamine (2HCl), 44.7; N-p-biphenylyl-2-morpholinoethylamine (2HCl), 74.9; 4-(2-diethylaminoethoxy)biphenyl, 104; 4-benzylamino-4'-dimethylaminobiphenyl (2HCl), 45.0. Other compds. for which k is given are: N'-4-bi-phenylyl-N,N-diethyl-N,N',N'-trimethylethylenediammonium diiodide, 0.065; N-p-biphenylyl-N-methyl-2-morpholinoethylamine dimethiodide, 0.16; 4-(2-diethylaminoethoxy)biphenyl methiodide, 0.12; and p-biphenylyltrimethylammonium iodide, 0.04. UV absorption maxima are listed for all the salts except for 2-aminochrysene-HCl.

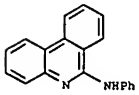
IT 62764-43-6, Phenanthridine, 6-amino-, hydrochloride (partition between paraffin oils and phosphate buffer)
RN 62764-43-6 CA
CN 6-Phenanthridinamine, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

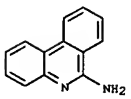
L8 ANSWER 70 OF 77 CA COPYRIGHT 2005 ACS on STN (Continued)

L8 ANSWER 71 OF 77 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 47:51952 CA
ORIGINAL REFERENCE NO.: 47:8829b-c
TITLE: The antiviral action of phenanthridinium compounds
AUTHOR(S): Dickinson, Lois; Chantrill, B. H.; Inkley, G. W.; Thompson, Mildred J.
CORPORATE SOURCE: Boots Pure Drug Co., Ltd., Nottingham, UK
SOURCE: British Journal of Pharmacology and Chemotherapy (1953), 8, 139-42
CODEN: BJPCAL; ISSN: 0366-0826
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB Twenty-three phenanthridines and diazapyrenes were tested against influenza A virus in eggs, against Pb phage of Pseudomonas aeruginosa and against a range of gram-pos. and gram-neg. bacteria. Many compds. possessed marked antiphage action, up to 1000 times that on the bacterial host. Several compds., active against phage, possessed slight antiinfluenza activity in eggs but the most promising compds. were inactive in mice. Seven of 9 compds. had a suppressive action against Rous sarcoma virus in chicks but only at a toxic dose.
IT **846-62-8**, Phenanthridine, 6-anilino-
(antiviral action of)
RN 846-62-8 CA
CN 6-Phenanthridinamine, N-phenyl- (9CI) (CA INDEX NAME)



L8 ANSWER 72 OF 77 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 47:51570 CA
ORIGINAL REFERENCE NO.: 47:8750h-i,8751a-b
TITLE: New syntheses of heterocyclic compounds. XVIII. 2,10-Diazaphenanthrenes by application of the Stieglitz rearrangement
AUTHOR(S): Berg, S. S.; Petrow, V.
CORPORATE SOURCE: May & Baker, Ltd., Dagenham, UK
SOURCE: Journal of the Chemical Society, Abstracts (1952) 3713-16
CODEN: JCSAAZ; ISSN: 0590-9791
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB cf. C.A. 47, 6943e. 6-Phenylphenanthridine (C.A. numbering) (2.2 g.) and KNH2 (from 0.5 g. K) in 10 ml. liquid NH3, 48 hrs. at room temperature (sealed tube), give 600 mg. 6-aminophenanthridine, m. 188-90°. 1,3-Dimethyl-2-azafluoren-9-one (1,3-dimethyl-9H-indeno[2,1-c]pyridin-9-one) (58 g.), added (30 min.) to PhMgBr (87 g. PhBr) in 150 ml. ether, the mixture refluxed 1 hr., the cooled product diluted with 100 ml. ether, the Mg complex decomposed by refluxing 10 min. with 5 l. 2N H2SO4, and the base extracted with ether, gives 52% 1,3-dimethyl-9-phenyl-2-azafluoren-9-ol (I), m. 183-4°. I (15 g.), 15 g. PCl5, and 100 ml. PhMe, carefully mixed and refluxed 30 min., give 14 g. 9-chloro-1,3-dimethyl-9-phenyl-2-azafluorene (II), m. 114-16°. II (10 g.) and KNH2 (1.3 g. K) in 25 ml. liquid NH3 (3 days at room temperature) give 2.1 g. of the 9-NH2 compound (III), pale brown, m. 116-20° (picrolonate, yellow, m. above 280°). III (2.9 g.) in 75 ml. EtOH containing 700 mg. dry HCl, treated (1 hr.) at 0-5° with 20 ml. freshly prepared N KOCl, gives the 9-chloroamino compound (IV), pale yellow, m. 125-8°. IV (2 g.) in 20 ml. anhydrous C5H5N, treated with 2 g. anhydrous MeONa and kept overnight, gives 400 mg. (20%) 1,3-dimethyl-9-phenyl-2,10-diazaphenanthrene (2,4-dimethyl-6-chloro-3,5-phenanthroline) (V), m. 129-31°; with KNH2 in liquid NH3 2 g. V yields 450 mg. 9-amino analog (VI), pale brown, m. 187-9°. III (3 g.), 1.6 g. KNO3, and KNH2 (2 g. K) in 20 ml. liquid NH3 containing 50 mg. Fe(NO3)3, 5 days at room temperature, give 300 mg. of the picrate of VI. This synthesis of VI avoids the danger involved in the use of HN3 (cf. P., C.A. 40, 4379.9).
IT **832-68-8**, Phenanthridine, 6-amino-
(preparation of)
RN 832-68-8 CA
CN 6-Phenanthridinamine (9CI) (CA INDEX NAME)

L8 ANSWER 72 OF 77 CA COPYRIGHT 2005 ACS on STN (Continued)



L8 ANSWER 73 OF 77 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 46:14706 CA
ORIGINAL REFERENCE NO.: 46:2583b-c
TITLE: Heterocyclic quaternary ammonium compounds
INVENTOR(S): Sprague, James M.
PATENT ASSIGNEE(S): Sharp & Dohme, Inc.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2567912		19510911	US	

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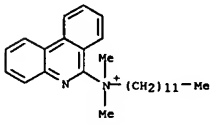
AB Quaternary ammonium compds. from Me2 (C12H25)N and RCH2X, where R is a 2-benzimidazolyl, 1-methyl-2-benzimidazolyl, or 6-phenanthridyl group and X is a halogen, are potent antibacterial agents. Dimethyldodecyl(2-benzimidazolylmethyl)ammonium chloride (I) m. 102.5-4°; 1-methyl-2-benzimidazolylmethyl analog m. 122-3°; (6-phenanthridylmethyl) analog m. 77-9°; ammonium hydroxide analog of I m. 120-1°. Other anion salts are mentioned without data.
IT **857168-43-5**, Ammonium, dodecyldimethyl-6-phenanthridinyl-, chloride
(preparation of)
RN 857168-43-5 CA
CN Ammonium, dodecyldimethyl-6-phenanthridinyl-, chloride (5CI) (CA INDEX NAME)



● Cl⁻

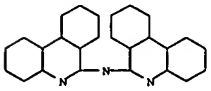
L8 ANSWER 74 OF 77 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 45:52921 CA
ORIGINAL REFERENCE NO.: 45:9061a-h
TITLE: New syntheses of heterocyclic compounds. XII. The condensation of ethyl β-aminocrotonate with some cyclic amidines
AUTHOR(S): Antaki, H.; Petrow, V.
CORPORATE SOURCE: Univ. London
SOURCE: Journal of the Chemical Society, Abstracts (1951) 551-5
CODEN: JCSAAZ; ISSN: 0590-9791
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB cf. C.A. 44, 2531i. MeC(NH2); CHCO2Et (I) and 9.4 g. 2-aminopyrimidine (II), heated 6-8 hrs. at 160-80° and 1 hr. at 200-20°, give 4,4a-dihydro-4-keto-2-methyl-1,4a-diazanaphthalene (III) (C.A. numbering), m. 124-5° (hydrate, m. 104-5°; picrate, yellow, m. 184°); this was considered the 4-Me derivative by Crippa and Scevola (C.A. 32, 166.6). I (5 g.), 6 g. 2-bromopyrimidine, 5 g. anhydrous K2CO3, and 100-200 mg. Cu bronze, heated 5-6 hrs. at 180-200°, also give III. II (9.4 g.) and 26 g. AcCH2-CO2Et, heated 4 hrs. at 100°, give 2-acetoacetamidopyrimidine, m. 112-13°; concentrated H2SO4 (24 hrs. at room temperature). gives III. I (8.5 g.) and 7 g. 2-amino-4-methylpyridine, 8 hrs. at 180-200°, give 1,4-dihydro-4-keto-2,7-dimethyl-1,4a-diazanaphthalene, m. 137° (picrate, yellow, m. 198°). 4,4a-Dihydro-4-keto-2,8-dimethyl-1,4a-diazanaphthalene, m. 130° [picrate, yellow, m. 190° (decomposition)]. I (12 g.) and 10 g. 2-amino-6-methylpyridine, heated 7-8 hrs. at 190° and 2 hrs. at 210-20°, gives 1,3-bis(6-methyl-2-pyridyl)urea, m. 194° [picrate, yellow, m. 190° (decomposition)]. 2-Aminoquinoline (5 g.) and 5 g. I, heated 6 hrs. at 180-200°, give 1,3-di-2-quinolylurea, m. 286°. 2-Chloroquinoline (5 g.), 4 g. I, 5 g. anhydrous K2CO3, and a trace of Cu bronze, heated 3 hrs. at 190° and 1 hr. at 200-20°, give 4,4a-dihydro-4-keto-2-methyl-1,4a-diazaphenanthrene, pale yellow, m. 131° (picrate, yellow, m. 207°). 6-Aminophenanthridine (C.A. numbering) gives 6,6'-diphenanthridylamine (?), yellow, m. above 310°. 2-Aminothiazole and I give 3a,4-dihydro-4-keto-6-methyl-3a,7-diazathianaphthene, pale yellow, m. 130°; it does not form a picrate but yields a H2O-soluble HCl salt and sulfate; methiodide, m. 304° (decomposition): nitrate, pale yellow, m. 148° (decomposition); x-NO2 derivative, yellow brown, m. 165°. 2-Amino-4-methylthiazole and I give 3a,4-dihydro-4-keto-3,6-dimethyl-3a,7-diazathianaphthene, pale yellow, m. 136°. 2-Aminobenzothiazole and I yield 4,4a-dihydro-4-keto-2-methyl-1,4a-diaza-9-thiafluorene, m. 199°; 7-acetamido derivative, m. 290° [the 7-NH2 derivative yields a, di-HCl salt, with 1 mol. H2O, yellow brown, m. above 266° (decomposition)]; 7-carbethoxy derivative, m. 204-6°; 7-Cl derivative, pale yellow, m. 220°; 7-EtO derivative, m. 198°. 2-Aminonaphtho[2',1':4,5]thiazole and I give 4,4a-dihydro-4-keto-2-methyl-7,8-benzo-1,4a-diaza-9-thiafluorene, m. 207°, and 2-aminobenzoxazole (IV) yields 4,4a-dihydro-4-keto-2-methyl-1,4a-diaza-9-oxafluorene, m. 146°. IV and Et 2-ketocyclohexanecarboxylate (V) (1 hr. at 180-200°) yield 4,4a-dihydro-4-keto-2,3-cyclohexeno-1,4a-diazo-9-oxafluorene, m. 198°. 2-Aminobenzimidazole (VI) and IV or AcCH2CO2Et give 4,4a-dihydro-4-keto-2-methyl-1,4a-triazafluorene (VII), m. 294° (decompn.) (9-Ac deriv., m. 168°). VI and AcCHEtCO2Et (heated at 130-40°) give the 3-Et deriv. of VII, m. 284° (decompn.); 3-Pr analog, m. 253°; 3-iso-Pr analog, m. 294°. VI and V, heated at 100° until the mixt. liquifies and then at 150-60° until it solidifies, give 4,4a-dihydro-4-keto-2,3-cyclohexeno-1,4a,9-triazafluorene, m. 296° (methiodide, decomp. about 228°). VI and Et cyclopentanecarboxylate give 4,4a-dihydro-4-keto-2,3-cyclopenteno-1,4a,9-triazafluorene, m. 304°. VI (1.3 g.) and 0.83 g. MeC(NH2): CHCN, heated at 180°, give 4,4a-dihydro-4-imino-2-methyl-1,4a,9-triazafluorene, m. above 300°; the 2-Ph analog, yellow, m. above 300°.

IT 95953-05-2, Phenanthridine, 6,6'-iminodi- (preparation of)

RN 95953-05-2 CA

CN Phenanthridine, 6,6'-iminodi- (7CI) (CA INDEX NAME)



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

L8 ANSWER 75 OF 77 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 43:6478 CA
ORIGINAL REFERENCE NO.: 43:1417e-i,1418a-i,1419a-i,1420a-i,1421a
TITLE: Some syntheses in the benzoquinoline, benzacridine, and phenanthridine series
AUTHOR(S): Albert, Adrien; Brown, D. J.; Duewell, Heinz
SOURCE: Journal of the Chemical Society, Abstracts (1948) 1284-95
CODEN: JCSAAZ; ISSN: 0590-9791
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 43:6478

GI For diagram(s), see printed CA Issue.

AB The following compds. were prepared to demonstrate the relation between antibacterial activity and the extent of cationic ionization at pH 7; however, no such data are given in the present paper. In general, the NH2 compds. were prepared by heating 2 g. of the Cl compound and 6-10 g. PhOH or p-MeC6H4OH 4 h. at 180° while passing NH3 through at the rate of 2 bubbles/s.; the product is made alkaline to orange-II paper with NaOH and the precipitate repeatedly extracted with dilute AcOH; the exts., adjusted to pH 6, filtered, and made strongly alkaline, give the desired amide. 4-Chloro-5,6-benzoquinoline gives 75% of the 4-NH2 derivative, m. 149-50°; 4-amino-7,8-benzoquinoline, m. 173-4°, 75%. 4-Hydroxy-2-methyl-5,6-benzoquinoline (2 g.) and 6 mL. POCl3, refluxed 1 h. and the sticky residue stirred with ice and NH4OH, give 85% of the 4-Cl compound (I), m. 99-100°; with p-MeC6H4OH, I yields 95% of the 4-p-tolyloxy compound, m. 137°. I (5 g.), 20 g. Ph2O, and 0.5 g. anhydrous CuSO4 at 200°, treated 4 h. with NH3, give 90% 4-amino-2-methyl-5,6-benzoquinoline, m. 164° (corrected). 3,2-H2NC10H6CO2Et (35 g.) and 70 mL. Ac2O, heated 10 min. at 90°, give 36 g. of the Ac derivative (II), m. 123-4°; 25 g. II and 25 mL. POCl3, heated about 0.5 h. at 75° and during 90 min. to 125°, the product slowly stirred into 100 mL. H2O, the mixture heated 5 h. in a boiling water bath, the dried solid extracted with 250 mL. EtOH, the insol. portion extracted with N Na2CO3 and H2O, and the acid portion purified through the Na salt, give 55% N-(2-carboxy-3-naphthyl)-4-hydroxy-2-methyl-6,7-benzoquinoline-3-carboxamide (III), pale yellow, amorphous, with 0.5 mol. H2O, soluble in C5H5N with salt formation and in (CH2OH)2 with decarboxylation. The EtOH filtrate yields a slimy orange acidic substance [m. about 190° (decomposition)] which, on acid hydrolysis at 210°, yields only 3,2-H2NC10H6CO2H (IV) and AcOH; this is apparently an anhydride of IV. Crude III, heated 3 h. with 75 mL. H2SO4 and 75 mL. H2O at 210°, gives 60% 4-hydroxy-2-methyl-6,7-benzoquinoline (V), buff, m. 296-8°; the solns. in H2O, EtOH, and C5H5N are pale yellow with intense violet fluorescence; the acid and alkaline solns. are yellow with a green fluorescence. The crude chloride from V yields 4-amino-2-methyl-6,7-benzoquinoline, pale yellow, m. 180°; the EtOH or Me2CO solution is yellow with intense blue fluorescence. 4-Amino-2-methyl-7,8-benzoquinoline, m. 149-50°, 70%. 3-Nitro-4-hydroxyquinoline (3.45 g.) and 20 mL. POCl3, refluxed 2 h., 4-chloro-3-nitroquinoline, cream, m. 119-20°; this yields 90% 3-nitro-4-aminoquinoline, bright yellow, m. 261-2°. 3,2-H2NC10H6CO2H (9.17 g.) and 275 mL. N HCl, treated at 60° with NaO2N:CHCHNONa (from 6.03 g. MeNO2), gives 85% 3-(2-nitroethylideneamino)-2-naphthoic acid, yellow, m. 213° (decompn.); with Ac2O and AcONa this yields 50% 3-nitro-4-hydroxy-6,7-benzoquinoline, m. above 300° (decompn.); POCl3 gives 90% of the 4-Cl compd., orange, m. 237° (decompn.); 3-nitro-4-amino-6,7-benzoquinoline (VI), orange, m. 282-3°, sol. in 700 parts EtOH at 0° and in 800 parts Me2CO at 20°; the HCl salt is less sol. than 1 part in 5000 parts cold H2O. VI (6.4 g.), 23.3 g. SnCl2, 45 mL. concd. HCl, 15 mL. H2O, and 100 mL. EtOH, refluxed 2 h., give 90% 3,4-diamino-6,7-benzoquinoline, m. 212° (decompn.); it is readily oxidized in the air and was analyzed as the di-HCl salt (VII), with 2 mols. H2O, bright yellow, m. about 310° (decompn.), very sol. in H2O to an orange soln. with intense green fluorescence; phenanthrenequinone gives an azine, m. about 370°, which forms an intense green soln. in H2SO4. VII (0.56 g.) in 5 mL. H2O, stirred at -5° with 5 mL. N HCl at -5° and then treated (5 min.) with 0.15 g. NaNO2 in 5 mL. H2O, gives 80% 3,4-triazolo-6,7-benzoquinoline, cream, m. about 290° (decompn.); it is sol. in about 300 parts boiling EtOH; the yellow dil. soln. has a green fluorescence; the H2SO4 soln. is blood-red. 1,2-ClC10H6NH2 and AcCH2CO2Et, kept over H2SO4 5 days, give 90% of Et β-(1-chloro-2-naphthylamino)crotonate, which, slowly added to paraffin at 270° and heated for 15 min., gives 55% 8-chloro-4-hydroxy-2-methyl-6,7-benzoquinoline, m. above 350°; the crude Cl deriv. (m. 159-61°) yields 65% 8-chloro-4-amino-2-methyl-6,7-benzoquinoline, brownish yellow, m. 179-80°. 4-Quinolinol, on nitration and redn., gives 6-amino-4-quinolinol, m. 242° (decompn.); this was transformed to 1-hydroxy-p-phenanthroline by the method of Kermack and Weatherhead (C.A. 34, 7911.5); through the Cl deriv. this yields 85% 1-amino-p-phenanthroline, m. 204°. 3,2-H2NC10H6CO2H (8 g.) and 8 g. cyclohexanone, slowly heated (0.5 h.) to 210°, heated 1.5 h. at 210-20°, and the product extd. with 60 mL. C6H6, give 50% 9-hydroxy-5,6,7,8-tetrahydro-2,3-benzacridine (C.A. numbering for acridine nucleus), yellow, m. 315°; POCl3 gives 85% of the 9-Cl compd., cream, m. 141-2°, and this yields 75% of the 9-NH2 compd., orange-yellow, m. 236-8°, sol. in 55 parts boiling and 400 parts ice-cold PhMe, shows an intense blue fluorescence in EtOH, and its HCl salt (VIII) dissolves in 500 parts cold H2O with pale yellow color and blue fluorescence. A 0.2% soln. of VIII, exposed to direct sunlight 2 days, gives 95% of the polymer, (C17H16N2)n, m. 265°; the polymn. is not reversed by irradn. with light of 3650 A. 9-Chloro-3,4-benzacridine (11 g.) in 54 g. PhOH at 70°, treated with 6 g. (NH4)2CO3 (5 min.), the mixt. heated 0.5 h. at 120°, the melt poured into NaOH, the base extd. with 300 mL. N AcOH, the pH adjusted to about 6, and the filtrate made alk., gives 90% 9-amino-3,4-benzacridine, yellow, m. 196-7°; the pale yellow EtOH soln. has an intense violet fluorescence (von Braun, C.A. 21, 1122, ascribed this structure to a compd. m. 94-8°); the pale yellow HCl salt is sol. in 150 parts cold H2O (the faint green fluorescence becomes intense violet on diln.). Details are given of the reaction of 3,2-HOC10H6CO2H and PhNH2 (10 h. at 120°) which yields 52% 3,2-HOC10H6CONHPh, 16% 3,2-PhNHC10H6CONHPh, and 28% 3,2-PhNHC10H6CO2H; the last with POCl3 gives 97% 9-chloro-2,3-benzacridine which yields 75% of the 9-NH2 compd. (IX), scarlet, m. 231-2°, sol. in 17 parts EtOH (orange fluorescence) (prepd. in absence of daylight but not affected by light from a 100-w.

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incandescent lamp); Ac deriv., with 0.25 mol. H2O, m. about 230° (decompn.); the orange EtOH soln. has a slight green fluorescence; it is sol. in N NaOH (scarlet) and in 2 N AcOH (purple). IX (0.244 g.) in 1 mL. HCl and 200 mL. H2O, boiled 5 min. in the dark and exposed to light (8 h.), gives the polymer (C17H12N2.HCl.0.75-H2O)n, which, stirred 1 day with N NaOH, gives the free base, ivory, m. 310°. 9-Chloro-1,2-benzacridine yields 80% of the 9-NH2 compd., golden, m. 236-7°; the pale yellow EtOH soln. has a green fluorescence that becomes intense blue on diln.; the cream HCl salt dissolves in 400 parts cold H2O (violet fluorescence on diln.). 5,1-O2NC10H6NH2 (4 g.), 8 g. o-ClC6H4CO2K, 0.1 g. Cu, 1.5 g. anhyd. K2CO3, and 40 mL. cyclohexanol, heated 7 h. at 160-70°, the steam-distd. soln. adjusted to 300 mL., 30 g. K2CO3 added, and the K salt in 40 mL. boiling H2O acidified with AcOH, give 21% 2-(5-nitro-1-naphthylamino)benzoic acid, light brown, m. 239°; this yields 95% 9-chloro-4'-nitro-3,4-benzacridine which gives 85% 4'-nitro-9-amino-3,4-benzacridine (X), red, m. 250-2° (decompn.), sol. in about 120 parts cold Me2CO and 500 parts PhCl at 0°; hydrogenation of 1 g. X in 150 mL. Me2CO with Raney Ni at room temp. at atm. pressure gives 85% 4',9-diamino-3,4-benzacridine, orange-yellow, m. 225-6°, sol. in about 1000 parts PhCl at 0°; it is stable to boiling N NaOH; the mono-HCl salt is orange and the di-HCl salt is pale yellow. The general method for the prepn. of the 2-aminoquinoline analogs was to heat 3 g. of the Cl compd., 15 g. ZnCl2.2NH3, and 3 g. NH4Cl in an open tube contained in a sealed steel tube 6 h. at 220-40°; the product in HCl was pptd. with NH4OH to remove the Zn, extd. with N AcOH, the filtrate adjusted to pH 5 to ppt. unchanged Cl compd., and the base liberated with NaOH.
N-2-Naphthylacetoacetamide (XI) m. 102° (from C6H6) or 92° (from H2O); stirred 15 min. with 9 parts concd. HCl, it gives a quant. yield of 2-hydroxy-4-methyl-5,6-benzoquinoline which with POCl3 gives 95% of the 2-Cl compd.; this yields 60%. of 2-amino-4-methyl-5,6-benzoquinoline, m. 224-5°. AcCH2CO2Et (18 mL.) and 0.025 g. Cu(OAc)2 at 160°, treated with 5 g. 1-C10H7NH2 and the mixt. heated 15 min. at 160°, give 70% of the 1-isomer of XI, m. 115-17° (petr. ether) or 106-7° (C6H6); this yields 85% 2-hydroxy-4-methyl-7,8-benzoquinoline and 95% of the 2-Cl compd., which gives 40% 2-amino-4-methyl-7,8-benzoquinoline, m. 133-4°. CH2(CO2Et)2 (32 g.) at 180°, treated with 7.3 g. 1-C10H7NH2, the mixt. heated 15 min. at 180°, and the crude Et N-1-naphthylmalonamate (m. 227°) added to paraffin at 260-80°, gives 50% 2,4-dihydroxy-7,8-benzoquinoline; refluxed 2.5 h. with POCl3, it yields 80% 2,4-dichloro-7,8-benzoquinoline, m. 133°; this could not be aminated. 3,8-Dinitro-6(5H)-phenanthridone (C.A. numbering) (5 g.) and 50 mL. POCl3, refluxed 5 h., give 97% 6-chloro-3,8-dinitrophenanthridine, cream, m. 225°; amination gives 85% of the NH2 compd., yellow, m. 321-2°; redn. with SnCl2 in concd. HCl gives 70% 3,6,8-triaminophenanthridine, cream, m. 200°; the yellow EtOH soln. has an intense green fluorescence; it diazotizes to an orange soln. which gives a purple color with 2-C10H7OH. 4-Amino-2-methyl-6,7-benzoquinoline (5.01 g.) and 8.4 mL. Ac2O, refluxed 5 min. at 155°, 8.4 mL. BzH added, and the mixt. heated 3 h. at 155°, give 90%

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4-acetamido-2-styryl-6,7-benzoquinoline (XII), with 0.5 mol. H2O, yellow, m. 244°; 4.2 g. XII in 80 mL. C5H5N and 16 mL. H2O, treated (1 h.) with 5.3 g. KMnO4 (temp. below 20°), 30 mL. H2O added to keep the salts in soln., and the soln. stirred with addnl. H2O, gives 70% 4-amino-6,7-benzoquinoline-2-carboxylic acid; 1 g. of the acid, added to 60 mL. paraffin at 280 ± 2° (3 min.), gives 50% 4-amino-6,7-benzoquinoline, bright yellow, m. 233°; the yellow EtOH soln. has a blue fluorescence. 4-Chloro-2-methyl-6,7-benzoquinoline (1.14 g.) in 15 mL. MeOH contg. 0.23 g. Na, refluxed 2 h., gives 90% 4-methoxy-2-methyl-6,7-benzoquinoline (XIII), yellow, m. 103-5°; 1 g. XIII yields 1.3 g. of the crude styryl compd., oxidn. of which gives 4-methoxy-6,7-benzoquinoline-2-carboxylic acid, yellow, m. 255° (decompn.); demethylation by heating 3 h. at 210° with a mixt. of 3 mL. H2SO4 and 3 mL. H2O and the resulting product stirred 3 min. with paraffin at 270° give 4-hydroxy-6,7-benzoquinoline, cream, m. 272-3°; the C5H5N soln. has a violet fluorescence; the solns. in HCl and N NaOH are yellow with green fluorescence. 4-Chloro-3-nitro-6,7-benzoquinoline (3 g.) in 600 mL. CHCl3, treated with 2 g. p-MeC6H4SO2NHNH2 in 90 mL. CHCl3 and, after 24 h., the pptd. hydrazide (decomp. about 170°) heated 1.5 h. with 450 mL. 0.5 N NaOH, gives 60% 3-nitro-6,7-benzoquinoline (XIV), orange, m. 206°; redn. as above gives 85% 3-amino-6,7-benzoquinoline, yellow-brown, m. 240-1°; it is sol. in about 30 parts boiling EtOH, the soln. having an intense green fluorescence on diln. 6-Bromophenanthridine (1 g.) in 30 mL. EtOH and about 3 g. Raney Ni, added to 0.5 g. KOH in 10 mL. EtOH and shaken with H at room temp./atm. pressure, gives 95% phenanthridine (23 mL. of the EtOH could be replaced by 8 mL. C5H5N previously refluxed 4 h. with Raney Ni). 6(5H)-Phenanthridone (2 g.) in 150 mL. EtOH contg. 0.9 g. NaOH and 50 mL. H2O at 85°, treated (1.5 h., CO2 atm.) with 200 g. Na-Hg and the mixt. heated 1.5 h. at 100°, gives 1 g. of a hexahydro deriv., m. 176-8°. 7-Nitro-3,4-benzacridin-9(10H)-one (2.9 g.) in 150 mL. EtOH contg. 0.9 g. NaOH and 150 mL. H2O at 85°, treated (2 h., CO2 atm.) with 200 g. Na-Hg, the mixt. heated an addnl. 2 h., the EtOH removed, the residue extd. with 200 mL. boiling 1.5 N HCl, air blown through the ext. at 95° (4 h.), and the soln. filtered into 150 mL. 2.5 N NaOH, give 50% 7-amino-3,4-benzacridine, light brown, m. 165°, violet fluorescence in petr. ether and green in EtOH; the red mono-HCl salt gives an aq. soln. with a green fluorescence; the di-HCl salt is yellow. 3,2-H2NC10H6CO2H (9 g.), 15 g. p-BrC6H4NO2, 7.5 g. K2CO3, 0.3 g. Cu, and 45 mL. PhNO2, heated 1.5 h. at 150°, and 2 h. at 180°, give 3-p-nitroanilino-2-naphthoic acid (XV), yellow, m. 260°; POCl3, followed by hydrolysis with HCl, gives 7-nitro-2,3-benzacridine, with 0.5 mol. C5H5N, yellow-brown, does not m. at 360°; Na-Hg yields 60% 7-amino-2,3-benzacridine, bright red, m. 285-6°, sol. in 300 parts EtOH (intense orange fluorescence), stable to boiling N NaOH; the HCl salt is sol. in about 20 parts H2O (red). The m-NO2 isomer of XV, yellow, m. 226-7°, 15%. Distn. of 2,3-benzacridin-9(10H)-one with Zn dust gives only 15% 2,3-benzacridine but Na-Hg gives 70% [cf. Schopp, Ber. 27, 2840(1894)].
6,7-Benzoquinoline
results in 15% yield on heating 1 g. of the 1',2',3',4'-tetrahydro deriv. with 0.5 g. Pd-C in 5 mL. Ph2O 3 h. at 270°. 4,1-O2NC10H6NH2 (7.9 g.), 17 mL. concd. HCl, and 6.8 mL. (HCHO)3, heated 1 h. on the water bath, dild. with 1.5 l. 0.3 N HCl, boiled 0.5 h., the residue extd. with 3 more portions (1.5 l.) HCl, the base (pptd. with NH4OH) boiled 15 min. with 6 l. 0.3 N HNO3, and immediately pptd. with NH4OH, give 35% 6-nitro-2-methyl-7,8-benzoquinoline, light yellow, m. 141-2°; catalytic redn. in Me2CO over Raney Ni at room temp. and atm. pressure gives 90% 6-amino-2-methyl-7,8-benzoquinoline, m. 128-9°. 1'-Nitro-2-methyl-7,8-benzoquinoline (XVI), m. 153°, sol. in 50 parts cold Me2CO, 30%; 1'-NH2 compd., buff, m. 141-5°. 6-Nitro-2-styryl-7,8-benzoquinoline, yellow, m. 142-3°, 50%.

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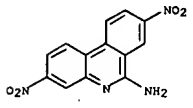
IT 855622-59-2, Phenanthridine, 6-amino-3,8-dinitro-
(preparation of)

RN 855622-59-2 CA

CN Phenanthridine, 6-amino-3,8-dinitro- (5CI) (CA INDEX NAME)



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ACCESSION NUMBER: 37:8471 CA
ORIGINAL REFERENCE NO.: 37:1432h-i,1433a-g
TITLE: A Hofmann-type rearrangement in liquid ammonia
AUTHOR(S): White, H. C.; Bergstrom, F. W.
SOURCE: Journal of Organic Chemistry (1942), 7, 497-507
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB Since it has been found that 2-phenyl-4-quinolinecarboxylic acid (I) when treated with KNH2 and KNO3 gives good yields of 2-phenylindole, the amide (II) of I, 2-(2-naphthyl)quinoline- (III), 2-(p-methoxyphenyl)quinoline- (IV), 2-phenylbenzo [h] quinoline- (V), 2-p-xenylquinoline-4-carboxamide (VI) and 3-phenylbenzo[f]quinoline-1-carboxamide (VII) are subjected to the same treatment. II, m. 195-7°, is prepared in 49.7% yield by refluxing 22.1 g. isatin, 16 g. NH4Cl, 180 cc. concentrated NH4OH and 20 g. PhAc for 50 min. III, prepared from the acid chloride, m. 250.5-1°; IV m. 245-6°; V, prepared in 67% yield, m. 268-9°; VI, m. 245.5-6° is prepared from the chloride of 2-p-xenyl-4-quinolinecarboxylic acid (VIII) which is obtained by refluxing 10 g. p-PhC6H4Ac and 9 g. isatin in 100 cc. 33% KOH for 5 hrs. After cooling, the mixture is acidified with AcOH, giving 11 g. VIII, m. 292-3°. VII, prepared in 81% yield, m. 239-40°. When 2.48 g. II and KNH2 from 1.17 g. K in liquid NH3 are kept at room temperature for 23 days, 43.4% 2-phenyl-4-aminoquinoline (IX), m. 163-4°, is formed. By using the same conditions but with addition of KNO3 or Hg, 89-98% IX is obtained in addition to a corresponding amount of KNO2 and KCNO. With Ba(NH2)2 in lieu of KNH2, II gives 2-phenylquinoline as chief product. 2-Phenyl-6-methyl-4-quinolinecarboxamide, KNH2 and KNO3 kept at room temperature for 4 days give a reddish brown tar from which 2-phenyl-4-amino-6-methylquinoline, m. 184-5°, is isolated. V, KNH2 and KNO3 give 54% 2-phenyl-4-aminobenzo[h]quinoline, m. 162.5-3°. The NHMe or NMe2 derivative of I with KNH2 and KNO3 gives IX in 70.5% and 23.3% yield, resp. o-BzC6H4CONH2, KNH2 and KNO3 at 20° for 6 days give 20% o-BzC6H4NH2, m. 105-7°, and 51% KNO2. 2-p-Tolyl-4-quinolinecarboxamide, III, IV and VI with KNH2 and KNO3 give only tars. PhCH2CONH2 dissolves in KNH2 and liquid NH3 with a deep red color, probably due to the formation of PhCHKCONHK, and after treatment with KNO3 up to 74% is recovered without formation of any KNO2. C18H35CONH2 and 2-propyl-2-phenyl-4-methylpentanamide do not react with KNH2 and KNO3. 4-Quinolinecarboxamide, KNH2 and KNO3 kept for 2 days give 54% 2-amino-4-quinolinecarboxamide (X), m. 218-18.5°; picrate m. 278-80° (decomposition). Saponification of X gives the acid, m. 349-53°. The results indicate that the reaction occurs only if the CONH2 group is activated by CO or CN at a favorable position in the mol. When 0.71 g. 2-phenyl-4-quinolyl isocyanate (XI), 0.4 g. KNO3 and KNH2 from 0.35 g. K are allowed to react for 2 days, 77% of XI is recovered, but with 5 equivalent KNH2 and 1 equivalent KNO3 for 36 hrs., 62% XI and 20% IX are obtained. 2-Phenyl-6-methyl-4-quinolyl isocyanate (XII), prepared according to John (C. A. 25, 5427), m. 246-7° instead of 214° as reported; picrate m. 206-7°. XII, KNH2 and KNO3 after 2 days at room temperature are recovered unchanged. PhNCO (XIII) in liquid NH3 gives 87.5%

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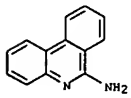
PhHNCONH2, m. 144-5°, while addn. of KNH2 gives (PhHN)2 CO, m. 233-4°. 1-C10H7NCO (XIV) and KNH2 in liquid NH3 at -33° give 48% 1-C10H7HNCONH2 (XV), m. 211-12°, and 38% (1-C10H7HN)2CO (XVI), m. 283-5°. When to 1-C10H7NHK from 4 g. amine in liquid NH3, 4 g. XIV is slowly added and the reaction stopped after 10 min. by addn. of NH4Cl, 55% XV and 38% XVI are formed. When 0.384 g. HCONH2, 1.1 g. KNO3 and KNH2 from 0.7 g. K are kept for 18 hrs. in a sealed tube, 176.6 cc. gas, contg. 97.5% H, is formed. 9-Amino-9-phenylfluorene, KNH2 and KNO3 give 61% 9-aminophenanthridine, m. 190-0.5°. Ph3CNH2, KNH2 and KNO3 at 80° for 14 hrs. in a steel bomb give 43% BzNH2. Apparently a Stieglitz-type rearrangement takes place with the formation of Ph2C:NPh, which is split to PhC(:NH)NHK and this is hydrolyzed to BzNH2. The mechanisms of these reactions are discussed.

IT 832-68-8, Phenanthridine, 6-amino-
(preparation of)

RN 832-68-8 CA

CN 6-Phenanthridinamine (9CI) (CA INDEX NAME)



L8 ANSWER 77 OF 77 CA COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 32:33042 CA

ORIGINAL REFERENCE NO.: 32:4588c-i,4589a-f

TITLE: Phenanthridine series. V. The color and antiseptic properties of quaternary salts

AUTHOR(S): Morgan, Gilbert T.; Walls, Leslie P.; Browning, C. H.; Gulbransen, R.; Robb, J. V. M.

SOURCE: Journal of the Chemical Society, Abstracts (1938) 389-97
CODEN: JCSAAZ; ISSN: 0590-9791

DOCUMENT TYPE: Journal

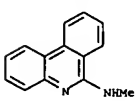
LANGUAGE: Unavailable

AB cf. C. A. 30, 103.5. The work reported in parts I and II (C. A. 26, 461, 5956) drew attention to the color of certain quaternary salts of the series, which also contained primary NH2 groups. Further information has been obtained by replacement of the latter by tert-NH2 groups and by the study of other series of salts. 3-Amino-9-methylphenanthridine (I) yields a HCl salt, yellow, with 2 mols. H2O. I and MeI, heated at 150° for 6 h., give 3-dimethylamino-9-methylphenanthridine, brown, m. 146°; pure quaternary salts could not be obtained therefrom by further methylation; HCl salt, red needles. 3-Acetamido-9,10-dimethylphenanthridinium methosulfate and KI give the iodide, yellow needles; AgCl gives the chloride, pale yellow needles, with 1 mol. H2O. 9-p-Aminophenylphenanthridine (II) yields a red mono-HCl salt; II with MeI at 150° for 8 h. gives 9-p-dimethylaminophenylphenanthridine (III), buff, m. 179-81°; HCl salt, orange-red, transparent plates. 9-p-Aminophenyl-10-methylphenanthridinium iodide (IV), ruby-red, transparent prisms. p-Acetamidophenyl-10-methylphenanthridinium chloride, pale orange prisms, with 2 mols. H2O. Heating III with p-MeC6H4SO3Me in PhNO2 at about 180° gives a dark red solution, from which a white p-toluenesulfonate seps.; this was converted into 9-phenanthridyl-p-phenyltrimethylammonium iodide, m. 179° (decomposition); the red melt solidified and then m. 235° (conversion into an isomer(?)); the red aqueous liquor after steam distillation of PhNO2 gives 9-p-dimethylaminophenyl-10-methylphenanthridinium p-toluenesulfonate, with 2 mol. H2O, m. with loss of H2O at 120°, forming a dark red glass; iodide (V), brick-red prisms, m. 238° (decomposition); chloride, hydrated ruby-red prisms, with Cu reflex. When III is methylated with Me2SO4 a diquaternary dimethosulfate is formed, characterized as the diiodide (VI), pale yellow prisms, m. 232-6° (decomposition); the same salt was obtained in high yield when a large excess of p-MeC6H4SO3Me was used; the white chloride lost MeCl slowly at 100° to yield the red monochloride. Heating IV with MeI at 180° for 7 h. gives V and VI. In this series the bases, primary and tertiary, and Ac derivs. are colorless or almost so, but monoacid salts and those with the hetero-N alone quaternary are red. The appearance of color is always associated with the possibility of tautomerism, probably due to wave-mech. resonance. In the synthesis of phenanthridine derivs. from acyl-o-xenylamines by POCl3 considerable resinification may occur, probably due to a side reaction involving elimination of the acyl group. The side reaction predominates when R in 4-R'C6H4C6H3(NHCOR)-2-R''-5 is Me, R' is NO2 and R'' is H or NO2; if R is Ph or p-O2NC6H4 the side reaction is suppressed and ring closure occurs, though very slowly. 5,2-O2N(H2N)C6H3Ph and p-O2NC6H4COCl in C5H5N give 5-nitro-2-p-nitrobenzamidobiphenyl, buff, m. 209°; refluxing with POCl3 for 30 h. gives 3-nitro-9-p-nitrophenyl-phenanthridine, pale yellow, m. 294°; catalytic redn. gives the 3-amino-9-p-aminophenyl deriv., m. 233°; HBr salt, with 1 mol. H2O, orange plates; sulfate, cream needles; di-Ac deriv., m. 327-8° (decompn.); p-MeC6H4SO3Me in PhNO2 gives the pale orange p-toluenesulfonate, converted to 3-acetomido-9-p-acetamidophenyl-10-methylphenanthridinium chloride, pale yellow needles; the free di-NH2 chloride, with 0.5 mol. H2O, forms transparent, red prismatic needles. The following were prepd. in substantially the same way as their isomers. 4'-Nitro-2-p-nitrobenzamidobiphenyl, m. 208°; 7-nitro-9-p-nitrophenylphenanthridine, m. 327°; 7-amino-9-p-aminophenyl deriv., pale yellow, m. 212°; the red HCl salt is extremely sol. in H2O; the sulfate forms brick-red talc-like crystals; di-Ac deriv., m. 172-3°. 7-Acetamido-9-p-acetamidophenyl-10-methylphenanthridinium p-toluenesulfonate, yellow needles or transparent prisms; chloride, with 1.5 mol. H2O, yellow prisms; the free di-NH2 chloride, with 0.5 mol. H2O, ruby-red, m. 262° (decompn.). 4'-Nitro-2-benzamidobiphenyl, m. 165.5°; 7-nitro-9-phenylphenanthridine, pale yellow, m. 237°. 5,4'-Dinitro-2-benzamidobiphenyl, m. 250°; it gives a very small yield of 3,7-dinitro-9-phenylphenanthridine, yellow, m. 275-7°. Heating 9-chlorophenanthridine (VI) and 33% MeOH-MeNH2, at 180° for 5 h. gives 9-methylaminophenanthridine, m. 187°; sulfate, needles, the 2% aq. soln. of which had PH 6-6.5; Ac deriv., m. 155°; 9-dimethylamino homolog (VII), m. 61.5°; HCl salt, needles, the 2% aq. soln. of which had PH 4.5-5. VI and Me3N, followed by KI, give 9-phenanthridyltrimethylammonium iodide, m. 234° (decompn.); the 2% aq. soln. has a PH of 5.5. VII and MeI, heated at 125° for 4 h., give 9-dimethylamino-10-methylphenanthridinium iodide, yellow, m. 230° (decompn.); heating the aq. soln. gives N-methylphenanthridone. 9-ω-Phenanthridylmethyltrimethylammonium iodide, m. about 222° (decompn.), results from 9-ω-chloromethylphenanthridine and MeNH2 at 100° for 2 h., followed by KI; C5H5N gives 9-ω-phenanthridylmethyl-N-pyridinium chloride (VIII), decomps. about 250°; the 2% aq. soln. had a PH of 6.5°; the nitrate, sulfate and perrhenate were sparingly sol. in H2O; piperidine gives 9-ω-piperidinomethylphenanthridine, pale yellow, m. 90-3°; HCl salt, with 1 mol. H2O, prisms; the 2% aq. soln. had pH 5.5. A report is given on the antiseptic action of 31 phenanthridine compds. and certain relations between constitution and action are discussed. VIII is among the most active members of the series for Staphylococcus and B. coli in serum as well as in aq. soln.

IT 951-07-5, Phenanthridine, 6-methylamino-
(preparation of)

RN 951-07-5 CA

CN Phenanthridine, 6-(methylamino)- (6CI, 7CI, 8CI) (CA INDEX NAME)



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L3         666 S L1 FULL

     FILE 'CA' ENTERED AT 15:38:01 ON 08 SEP 2005
L4         151 S L3
L5          90 S L4 AND PY<1999
L6          12 S L5 AND (PHARM? OR DRUG?)
L7          78 S L5 NOT L6
L8          77 S L7 AND PY<1998

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Executing the logoff script...


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